```
****************************Gaussian NBO Version 3.1*****************************
          N A T U R A L   A T O M I C   O R B I T A L   A N D
        N A T U R A L   B O N D   O R B I T A L   A N A L Y S I S
****************************Gaussian NBO Version 3.1*****************************

      /RESON  / : Allow strongly delocalized NBO set
      /PLOT   / : Write information for the orbital plotter

Analyzing the SCF density

Job title: Molden generated mol2

Storage needed:   7831912 in NPA,  10391205 in NBO,  17213248 in NLMO (  33504081 available)


NATURAL POPULATIONS:  Natural atomic orbital occupancies

  NAO  Atom  No  lang   Type(AO)    Occupancy      Energy
---------------------------------------------------------
    1    C    1  S      Cor( 1S)     1.99866      -9.74312
    2    C    1  S      Val( 2S)     0.91258      -0.15652
    3    C    1  S      Ryd( 3S)     0.00955       1.36430
    4    C    1  S      Ryd( 4S)     0.00076       2.34685
    5    C    1  S      Ryd( 5S)     0.00001      20.68659
    6    C    1  px     Val( 2p)     1.09440      -0.03788
    7    C    1  px     Ryd( 3p)     0.00150       1.01460
    8    C    1  px     Ryd( 4p)     0.00050       1.59088
    9    C    1  py     Val( 2p)     0.92636      -0.05262
   10    C    1  py     Ryd( 3p)     0.00146       0.90220
   11    C    1  py     Ryd( 4p)     0.00043       1.47200
   12    C    1  pz     Val( 2p)     0.90356      -0.01019
   13    C    1  pz     Ryd( 3p)     0.01427       1.24759
   14    C    1  pz     Ryd( 4p)     0.00080       1.55569
   15    C    1  dxy    Ryd( 3d)     0.00045       2.01034
   16    C    1  dxz    Ryd( 3d)     0.00223       2.42213
   17    C    1  dyz    Ryd( 3d)     0.00220       2.34682
   18    C    1  dx2y2  Ryd( 3d)     0.00032       2.03559
   19    C    1  dz2    Ryd( 3d)     0.00147       2.76860

   20    O    2  S      Cor( 1S)     1.99981     -18.41339
   21    O    2  S      Val( 2S)     1.69933      -0.76751
   22    O    2  S      Ryd( 3S)     0.00223       1.38071
   23    O    2  S      Ryd( 4S)     0.00003       6.03000
   24    O    2  S      Ryd( 5S)     0.00000      40.67539
   25    O    2  px     Val( 2p)     1.72668      -0.15911
   26    O    2  px     Ryd( 3p)     0.00513       0.79523
   27    O    2  px     Ryd( 4p)     0.00003       2.95877
   28    O    2  py     Val( 2p)     1.59521      -0.16678
   29    O    2  py     Ryd( 3p)     0.00349       0.75568
   30    O    2  py     Ryd( 4p)     0.00003       2.95301
   31    O    2  pz     Val( 2p)     1.57187      -0.20484
   32    O    2  pz     Ryd( 3p)     0.00205       0.66046
   33    O    2  pz     Ryd( 4p)     0.00015       3.08111
   34    O    2  dxy    Ryd( 3d)     0.00016       2.69838
   35    O    2  dxz    Ryd( 3d)     0.00127       2.97120
   36    O    2  dyz    Ryd( 3d)     0.00142       2.96156
   37    O    2  dx2y2  Ryd( 3d)     0.00015       2.71611
   38    O    2  dz2    Ryd( 3d)     0.00196       3.32929

   39    C    3  S      Cor( 1S)     1.99898      -9.73452
   40    C    3  S      Val( 2S)     0.92589      -0.18652
   41    C    3  S      Ryd( 3S)     0.00170       0.91213
   42    C    3  S      Ryd( 4S)     0.00042       2.03401
   43    C    3  S      Ryd( 5S)     0.00000      21.21279
   44    C    3  px     Val( 2p)     1.01149      -0.05903
   45    C    3  px     Ryd( 3p)     0.00297       0.88674
   46    C    3  px     Ryd( 4p)     0.00043       1.57562
   47    C    3  py     Val( 2p)     0.99048      -0.07465
   48    C    3  py     Ryd( 3p)     0.00244       0.81411
   49    C    3  py     Ryd( 4p)     0.00031       1.45698
   50    C    3  pz     Val( 2p)     1.03143      -0.03721
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51	C	3	pz	Ryd(3p)	0.00483	1.21918
52	C	3	pz	Ryd(4p)	0.00047	1.64524
53	C	3	dxy	Ryd(3d)	0.00057	2.44868
54	C	3	dxz	Ryd(3d)	0.00080	2.43860
55	C	3	dyz	Ryd(3d)	0.00077	2.27424
56	C	3	dx2y2	Ryd(3d)	0.00057	2.01657
57	C	3	dz2	Ryd(3d)	0.00066	2.45955
58	C	4	S	Cor(1S)	1.99875	-9.77297
59	C	4	S	Val(2S)	0.86758	-0.17193
60	C	4	S	Ryd(3S)	0.00124	0.95271
61	C	4	S	Ryd(4S)	0.00064	1.89448
62	C	4	S	Ryd(5S)	0.00000	21.52096
63	C	4	px	Val(2p)	0.99698	-0.06921
64	C	4	px	Ryd(3p)	0.00365	0.94114
65	C	4	px	Ryd(4p)	0.00059	1.71734
66	C	4	py	Val(2p)	0.98781	-0.08412
67	C	4	py	Ryd(3p)	0.00434	0.88173
68	C	4	py	Ryd(4p)	0.00050	1.67950
69	C	4	pz	Val(2p)	1.00925	-0.05448
70	C	4	pz	Ryd(3p)	0.00318	0.98410
71	C	4	pz	Ryd(4p)	0.00057	1.74149
72	C	4	dxy	Ryd(3d)	0.00065	2.48300
73	C	4	dxz	Ryd(3d)	0.00088	2.47737
74	C	4	dyz	Ryd(3d)	0.00078	2.28956
75	C	4	dx2y2	Ryd(3d)	0.00052	2.13935
76	C	4	dz2	Ryd(3d)	0.00096	2.48512
77	C	5	S	Cor(1S)	1.99898	-9.73846
78	C	5	S	Val(2S)	0.92415	-0.19176
79	C	5	S	Ryd(3S)	0.00175	0.95500
80	C	5	S	Ryd(4S)	0.00041	1.96130
81	C	5	S	Ryd(5S)	0.00000	21.12705
82	C	5	px	Val(2p)	1.01557	-0.05915
83	C	5	px	Ryd(3p)	0.00362	1.08553
84	C	5	px	Ryd(4p)	0.00028	1.55908
85	C	5	py	Val(2p)	1.00204	-0.08074
86	C	5	py	Ryd(3p)	0.00299	0.85095
87	C	5	py	Ryd(4p)	0.00023	1.41213
88	C	5	pz	Val(2p)	1.03476	-0.04874
89	C	5	pz	Ryd(3p)	0.00381	1.05069
90	C	5	pz	Ryd(4p)	0.00045	1.56944
91	C	5	dxy	Ryd(3d)	0.00061	2.36795
92	C	5	dxz	Ryd(3d)	0.00072	2.42356
93	C	5	dyz	Ryd(3d)	0.00069	2.23993
94	C	5	dx2y2	Ryd(3d)	0.00050	2.04986
95	C	5	dz2	Ryd(3d)	0.00079	2.49314
96	C	6	S	Cor(1S)	1.99909	-9.72700
97	C	6	S	Val(2S)	0.97286	-0.20262
98	C	6	S	Ryd(4S)	0.00097	1.40548
99	C	6	S	Ryd(3S)	0.00010	1.36155
100	C	6	S	Ryd(5S)	0.00000	21.24141
101	C	6	px	Val(2p)	1.04595	-0.06720
102	C	6	px	Ryd(3p)	0.00207	0.97039
103	C	6	px	Ryd(4p)	0.00038	1.33378
104	C	6	py	Val(2p)	1.03385	-0.08476
105	C	6	py	Ryd(3p)	0.00178	0.80232
106	C	6	py	Ryd(4p)	0.00052	1.21978
107	C	6	pz	Val(2p)	1.15908	-0.05534
108	C	6	pz	Ryd(4p)	0.00372	1.18812
109	C	6	pz	Ryd(3p)	0.00051	1.15498
110	C	6	dxy	Ryd(3d)	0.00057	2.41960
111	C	6	dxz	Ryd(3d)	0.00065	2.37515
112	C	6	dyz	Ryd(3d)	0.00047	2.23660
113	C	6	dx2y2	Ryd(3d)	0.00046	2.02376
114	C	6	dz2	Ryd(3d)	0.00061	2.40319
115	C	7	S	Cor(1S)	1.99920	-9.73026
116	C	7	S	Val(2S)	0.97727	-0.20593
117	C	7	S	Ryd(3S)	0.00079	1.07366

118	C	7	S	Ryd(4S)	0.00009	1.43879
119	C	7	S	Ryd(5S)	0.00000	21.18819
120	C	7	px	Val(2p)	1.07125	-0.06675
121	C	7	px	Ryd(3p)	0.00294	0.91731
122	C	7	px	Ryd(4p)	0.00029	1.35642
123	C	7	py	Val(2p)	1.05722	-0.08545
124	C	7	py	Ryd(3p)	0.00225	0.83594
125	C	7	py	Ryd(4p)	0.00031	1.38056
126	C	7	pz	Val(2p)	1.08023	-0.04985
127	C	7	pz	Ryd(3p)	0.00352	0.96811
128	C	7	pz	Ryd(4p)	0.00034	1.28696
129	C	7	dxy	Ryd(3d)	0.00050	2.35943
130	C	7	dxz	Ryd(3d)	0.00065	2.38376
131	C	7	dyz	Ryd(3d)	0.00053	2.19720
132	C	7	dx2y2	Ryd(3d)	0.00034	1.98427
133	C	7	dz2	Ryd(3d)	0.00078	2.45320
134	C	8	S	Cor(1S)	1.99910	-9.72396
135	C	8	S	Val(2S)	0.97448	-0.19933
136	C	8	S	Ryd(4S)	0.00096	1.40520
137	C	8	S	Ryd(3S)	0.00009	1.37585
138	C	8	S	Ryd(5S)	0.00000	21.31134
139	C	8	px	Val(2p)	1.11738	-0.06646
140	C	8	px	Ryd(3p)	0.00292	1.05382
141	C	8	px	Ryd(4p)	0.00043	1.22424
142	C	8	py	Val(2p)	1.04949	-0.08148
143	C	8	py	Ryd(3p)	0.00227	0.83420
144	C	8	py	Ryd(4p)	0.00050	1.21758
145	C	8	pz	Val(2p)	1.06886	-0.04826
146	C	8	pz	Ryd(3p)	0.00257	1.12803
147	C	8	pz	Ryd(4p)	0.00025	1.36733
148	C	8	dxy	Ryd(3d)	0.00052	2.37956
149	C	8	dxz	Ryd(3d)	0.00068	2.36251
150	C	8	dyz	Ryd(3d)	0.00054	2.25321
151	C	8	dx2y2	Ryd(3d)	0.00038	1.98804
152	C	8	dz2	Ryd(3d)	0.00063	2.50045
153	N	9	S	Cor(1S)	1.99944	-13.85291
154	N	9	S	Val(2S)	1.19090	-0.50288
155	N	9	S	Ryd(3S)	0.00124	1.33090
156	N	9	S	Ryd(4S)	0.00009	3.63900
157	N	9	S	Ryd(5S)	0.00000	30.09029
158	N	9	px	Val(2p)	1.34040	-0.22618
159	N	9	px	Ryd(3p)	0.00456	1.06628
160	N	9	px	Ryd(4p)	0.00017	2.51149
161	N	9	py	Val(2p)	1.29241	-0.23003
162	N	9	py	Ryd(3p)	0.00380	1.02328
163	N	9	py	Ryd(4p)	0.00022	2.56696
164	N	9	pz	Val(2p)	1.49693	-0.22348
165	N	9	pz	Ryd(3p)	0.00518	0.81343
166	N	9	pz	Ryd(4p)	0.00027	2.45311
167	N	9	dxy	Ryd(3d)	0.00081	2.68806
168	N	9	dxz	Ryd(3d)	0.00078	2.66768
169	N	9	dyz	Ryd(3d)	0.00075	2.50630
170	N	9	dx2y2	Ryd(3d)	0.00119	2.80409
171	N	9	dz2	Ryd(3d)	0.00057	2.59928
172	C	10	S	Cor(1S)	1.99868	-9.79306
173	C	10	S	Val(2S)	0.95163	-0.19674
174	C	10	S	Ryd(3S)	0.00282	1.54460
175	C	10	S	Ryd(4S)	0.00073	2.80549
176	C	10	S	Ryd(5S)	0.00001	20.18526
177	C	10	px	Val(2p)	1.02803	-0.07571
178	C	10	px	Ryd(4p)	0.00432	1.58590
179	C	10	px	Ryd(3p)	0.00112	1.48309
180	C	10	py	Val(2p)	0.88955	-0.04976
181	C	10	py	Ryd(3p)	0.00386	1.41902
182	C	10	py	Ryd(4p)	0.00131	1.47925
183	C	10	pz	Val(2p)	0.98089	-0.09841
184	C	10	pz	Ryd(3p)	0.00241	1.06237
185	C	10	pz	Ryd(4p)	0.00097	1.23892

186	C	10	dxy	Ryd(3d)	0.00063	2.50486
187	C	10	dxz	Ryd(3d)	0.00094	2.34896
188	C	10	dyz	Ryd(3d)	0.00080	2.05758
189	C	10	dx2y2	Ryd(3d)	0.00092	2.65358
190	C	10	dz2	Ryd(3d)	0.00066	2.25771
191	N	11	S	Cor(1S)	1.99943	-13.85452
192	N	11	S	Val(2S)	1.19030	-0.50308
193	N	11	S	Ryd(3S)	0.00128	0.91407
194	N	11	S	Ryd(4S)	0.00017	3.70645
195	N	11	S	Ryd(5S)	0.00000	30.34846
196	N	11	px	Val(2p)	1.33065	-0.22940
197	N	11	px	Ryd(3p)	0.00394	0.86395
198	N	11	px	Ryd(4p)	0.00015	2.48451
199	N	11	py	Val(2p)	1.27252	-0.22607
200	N	11	py	Ryd(3p)	0.00405	1.24960
201	N	11	py	Ryd(4p)	0.00024	2.65908
202	N	11	pz	Val(2p)	1.52689	-0.22548
203	N	11	pz	Ryd(3p)	0.00567	0.79387
204	N	11	pz	Ryd(4p)	0.00029	2.42763
205	N	11	dxy	Ryd(3d)	0.00110	2.85011
206	N	11	dxz	Ryd(3d)	0.00075	2.58149
207	N	11	dyz	Ryd(3d)	0.00063	2.50053
208	N	11	dx2y2	Ryd(3d)	0.00102	2.72328
209	N	11	dz2	Ryd(3d)	0.00065	2.58654
210	C	12	S	Cor(1S)	1.99902	-9.77380
211	C	12	S	Val(2S)	0.95156	-0.21206
212	C	12	S	Ryd(3S)	0.00127	1.08253
213	C	12	S	Ryd(4S)	0.00014	1.61045
214	C	12	S	Ryd(5S)	0.00001	21.53830
215	C	12	px	Val(2p)	1.11012	-0.07357
216	C	12	px	Ryd(3p)	0.00280	0.95340
217	C	12	px	Ryd(4p)	0.00073	1.48401
218	C	12	py	Val(2p)	0.91067	-0.07292
219	C	12	py	Ryd(3p)	0.00324	0.79780
220	C	12	py	Ryd(4p)	0.00074	1.43178
221	C	12	pz	Val(2p)	1.11138	-0.11675
222	C	12	pz	Ryd(3p)	0.00357	0.69544
223	C	12	pz	Ryd(4p)	0.00062	1.48102
224	C	12	dxy	Ryd(3d)	0.00078	2.68601
225	C	12	dxz	Ryd(3d)	0.00067	2.27755
226	C	12	dyz	Ryd(3d)	0.00097	2.13923
227	C	12	dx2y2	Ryd(3d)	0.00066	2.42726
228	C	12	dz2	Ryd(3d)	0.00052	2.21107
229	C	13	S	Cor(1S)	1.99902	-9.77360
230	C	13	S	Val(2S)	0.95045	-0.21104
231	C	13	S	Ryd(3S)	0.00126	1.07320
232	C	13	S	Ryd(4S)	0.00016	1.61680
233	C	13	S	Ryd(5S)	0.00001	21.53710
234	C	13	px	Val(2p)	0.90599	-0.07543
235	C	13	px	Ryd(3p)	0.00325	0.69990
236	C	13	px	Ryd(4p)	0.00068	1.39481
237	C	13	py	Val(2p)	1.17333	-0.06988
238	C	13	py	Ryd(3p)	0.00270	1.13719
239	C	13	py	Ryd(4p)	0.00079	1.58519
240	C	13	pz	Val(2p)	1.05485	-0.11765
241	C	13	pz	Ryd(3p)	0.00376	0.60073
242	C	13	pz	Ryd(4p)	0.00059	1.37186
243	C	13	dxy	Ryd(3d)	0.00064	2.53516
244	C	13	dxz	Ryd(3d)	0.00066	2.24298
245	C	13	dyz	Ryd(3d)	0.00060	2.15571
246	C	13	dx2y2	Ryd(3d)	0.00082	2.54005
247	C	13	dz2	Ryd(3d)	0.00077	2.18771
248	B	14	S	Cor(1S)	1.99770	-6.32115
249	B	14	S	Val(2S)	0.66358	0.05761
250	B	14	S	Ryd(3S)	0.00103	1.15216
251	B	14	S	Ryd(5S)	0.00046	8.65844
252	B	14	S	Ryd(4S)	0.00008	4.41273

253	B	14	px	Val(2p)	0.70960	0.13565
254	B	14	px	Ryd(3p)	0.00234	1.42385
255	B	14	px	Ryd(4p)	0.00119	1.56779
256	B	14	py	Val(2p)	0.66899	0.06300
257	B	14	py	Ryd(3p)	0.00127	0.93492
258	B	14	py	Ryd(4p)	0.00096	1.39166
259	B	14	pz	Val(2p)	0.88573	0.06457
260	B	14	pz	Ryd(3p)	0.00102	0.85270
261	B	14	pz	Ryd(4p)	0.00075	1.17255
262	B	14	dxy	Ryd(3d)	0.00071	2.07507
263	B	14	dxz	Ryd(3d)	0.00052	1.94055
264	B	14	dyz	Ryd(3d)	0.00056	1.47745
265	B	14	dx2y2	Ryd(3d)	0.00051	1.96939
266	B	14	dz2	Ryd(3d)	0.00064	1.72449
267	B	15	S	Cor(1S)	1.99698	-6.31152
268	B	15	S	Val(2S)	0.61819	0.10571
269	B	15	S	Ryd(3S)	0.00190	1.46089
270	B	15	S	Ryd(5S)	0.00047	7.59804
271	B	15	S	Ryd(4S)	0.00009	4.48440
272	B	15	px	Val(2p)	0.92413	0.09840
273	B	15	px	Ryd(3p)	0.00206	1.31720
274	B	15	px	Ryd(4p)	0.00130	1.48355
275	B	15	py	Val(2p)	0.76253	0.05368
276	B	15	py	Ryd(3p)	0.00155	0.86909
277	B	15	py	Ryd(4p)	0.00107	1.26480
278	B	15	pz	Val(2p)	0.84537	0.08837
279	B	15	pz	Ryd(3p)	0.00137	0.84774
280	B	15	pz	Ryd(4p)	0.00159	1.22861
281	B	15	dxy	Ryd(3d)	0.00032	1.95680
282	B	15	dxz	Ryd(3d)	0.00099	1.88291
283	B	15	dyz	Ryd(3d)	0.00057	1.76842
284	B	15	dx2y2	Ryd(3d)	0.00038	1.83587
285	B	15	dz2	Ryd(3d)	0.00056	1.94121
286	C	16	S	Cor(1S)	1.99875	-9.80721
287	C	16	S	Val(2S)	0.94763	-0.20470
288	C	16	S	Ryd(3S)	0.00328	1.57805
289	C	16	S	Ryd(4S)	0.00072	2.41066
290	C	16	S	Ryd(5S)	0.00001	20.13267
291	C	16	px	Val(2p)	0.96761	-0.06493
292	C	16	px	Ryd(4p)	0.00472	1.55252
293	C	16	px	Ryd(3p)	0.00138	1.43777
294	C	16	py	Val(2p)	0.96919	-0.09678
295	C	16	py	Ryd(4p)	0.00378	1.30532
296	C	16	py	Ryd(3p)	0.00098	1.28170
297	C	16	pz	Val(2p)	0.87817	-0.08117
298	C	16	pz	Ryd(3p)	0.00275	1.33929
299	C	16	pz	Ryd(4p)	0.00100	1.34000
300	C	16	dxy	Ryd(3d)	0.00067	2.22767
301	C	16	dxz	Ryd(3d)	0.00073	2.34673
302	C	16	dyz	Ryd(3d)	0.00062	2.55394
303	C	16	dx2y2	Ryd(3d)	0.00097	2.49251
304	C	16	dz2	Ryd(3d)	0.00098	2.13978
305	N	17	S	Cor(1S)	1.99942	-13.87230
306	N	17	S	Val(2S)	1.19577	-0.52154
307	N	17	S	Ryd(3S)	0.00148	0.92646
308	N	17	S	Ryd(4S)	0.00016	3.65502
309	N	17	S	Ryd(5S)	0.00000	30.34483
310	N	17	px	Val(2p)	1.29928	-0.24889
311	N	17	px	Ryd(3p)	0.00339	0.91215
312	N	17	px	Ryd(4p)	0.00018	2.53624
313	N	17	py	Val(2p)	1.39483	-0.24394
314	N	17	py	Ryd(3p)	0.00403	0.90304
315	N	17	py	Ryd(4p)	0.00021	2.50798
316	N	17	pz	Val(2p)	1.40171	-0.24450
317	N	17	pz	Ryd(3p)	0.00504	1.07403
318	N	17	pz	Ryd(4p)	0.00023	2.49052
319	N	17	dxy	Ryd(3d)	0.00082	2.59847
320	N	17	dxz	Ryd(3d)	0.00101	2.66011

321	N	17	dyz	Ryd(3d)	0.00081	2.80839
322	N	17	dx2y2	Ryd(3d)	0.00098	2.63634
323	N	17	dz2	Ryd(3d)	0.00065	2.48261
324	C	18	S	Cor(1S)	1.99904	-9.79245
325	C	18	S	Val(2S)	0.95409	-0.23008
326	C	18	S	Ryd(3S)	0.00122	1.09116
327	C	18	S	Ryd(4S)	0.00011	1.60526
328	C	18	S	Ryd(5S)	0.00001	21.50224
329	C	18	px	Val(2p)	1.14897	-0.08476
330	C	18	px	Ryd(3p)	0.00277	1.09505
331	C	18	px	Ryd(4p)	0.00077	1.46354
332	C	18	py	Val(2p)	0.96898	-0.11633
333	C	18	py	Ryd(3p)	0.00326	0.66051
334	C	18	py	Ryd(4p)	0.00064	1.32261
335	C	18	pz	Val(2p)	0.99460	-0.11442
336	C	18	pz	Ryd(3p)	0.00327	0.73971
337	C	18	pz	Ryd(4p)	0.00060	1.42469
338	C	18	dxy	Ryd(3d)	0.00066	2.38572
339	C	18	dxz	Ryd(3d)	0.00072	2.43996
340	C	18	dyz	Ryd(3d)	0.00051	2.42981
341	C	18	dx2y2	Ryd(3d)	0.00077	2.32009
342	C	18	dz2	Ryd(3d)	0.00087	2.06880
343	C	19	S	Cor(1S)	1.99904	-9.79308
344	C	19	S	Val(2S)	0.95531	-0.23143
345	C	19	S	Ryd(3S)	0.00119	1.11105
346	C	19	S	Ryd(4S)	0.00012	1.50559
347	C	19	S	Ryd(5S)	0.00001	21.48954
348	C	19	px	Val(2p)	0.87998	-0.08878
349	C	19	px	Ryd(3p)	0.00328	0.76182
350	C	19	px	Ryd(4p)	0.00069	1.32020
351	C	19	py	Val(2p)	1.10713	-0.11529
352	C	19	py	Ryd(3p)	0.00311	0.79488
353	C	19	py	Ryd(4p)	0.00079	1.34538
354	C	19	pz	Val(2p)	1.13364	-0.11509
355	C	19	pz	Ryd(3p)	0.00296	0.88114
356	C	19	pz	Ryd(4p)	0.00048	1.39859
357	C	19	dxy	Ryd(3d)	0.00079	2.38227
358	C	19	dxz	Ryd(3d)	0.00073	2.33511
359	C	19	dyz	Ryd(3d)	0.00064	2.46204
360	C	19	dx2y2	Ryd(3d)	0.00068	2.30207
361	C	19	dz2	Ryd(3d)	0.00063	2.15099
362	N	20	S	Cor(1S)	1.99942	-13.87362
363	N	20	S	Val(2S)	1.19344	-0.52341
364	N	20	S	Ryd(3S)	0.00137	0.93045
365	N	20	S	Ryd(4S)	0.00019	3.64246
366	N	20	S	Ryd(5S)	0.00000	30.34529
367	N	20	px	Val(2p)	1.29133	-0.24620
368	N	20	px	Ryd(3p)	0.00418	1.17239
369	N	20	px	Ryd(4p)	0.00019	2.60157
370	N	20	py	Val(2p)	1.42362	-0.24903
371	N	20	py	Ryd(3p)	0.00425	0.79774
372	N	20	py	Ryd(4p)	0.00023	2.44904
373	N	20	pz	Val(2p)	1.38809	-0.24958
374	N	20	pz	Ryd(3p)	0.00443	0.91796
375	N	20	pz	Ryd(4p)	0.00023	2.47273
376	N	20	dxy	Ryd(3d)	0.00081	2.60590
377	N	20	dxz	Ryd(3d)	0.00090	2.67443
378	N	20	dyz	Ryd(3d)	0.00080	2.79023
379	N	20	dx2y2	Ryd(3d)	0.00097	2.62359
380	N	20	dz2	Ryd(3d)	0.00078	2.47804
381	C	21	S	Cor(1S)	1.99873	-9.77771
382	C	21	S	Val(2S)	0.86755	-0.17742
383	C	21	S	Ryd(3S)	0.00123	1.05486
384	C	21	S	Ryd(4S)	0.00070	1.97609
385	C	21	S	Ryd(5S)	0.00000	21.10750
386	C	21	px	Val(2p)	1.03099	-0.09792
387	C	21	px	Ryd(3p)	0.00428	0.77589

388	C	21	px	Ryd(4p)	0.00056	1.65505
389	C	21	py	Val(2p)	0.99577	-0.06910
390	C	21	py	Ryd(3p)	0.00357	0.88429
391	C	21	py	Ryd(4p)	0.00066	1.67757
392	C	21	pz	Val(2p)	0.97205	-0.05564
393	C	21	pz	Ryd(3p)	0.00427	0.97499
394	C	21	pz	Ryd(4p)	0.00080	1.75403
395	C	21	dxy	Ryd(3d)	0.00064	2.42319
396	C	21	dxz	Ryd(3d)	0.00073	2.20192
397	C	21	dyz	Ryd(3d)	0.00097	2.56261
398	C	21	dx2y2	Ryd(3d)	0.00056	2.14439
399	C	21	dz2	Ryd(3d)	0.00088	2.57975
400	C	22	S	Cor(1S)	1.99897	-9.73706
401	C	22	S	Val(2S)	0.92100	-0.18700
402	C	22	S	Ryd(3S)	0.00226	0.88465
403	C	22	S	Ryd(4S)	0.00041	2.01434
404	C	22	S	Ryd(5S)	0.00000	21.04343
405	C	22	px	Val(2p)	0.97799	-0.08051
406	C	22	px	Ryd(3p)	0.00365	0.75667
407	C	22	px	Ryd(4p)	0.00034	1.51710
408	C	22	py	Val(2p)	1.01455	-0.05227
409	C	22	py	Ryd(3p)	0.00484	1.02652
410	C	22	py	Ryd(4p)	0.00041	1.64687
411	C	22	pz	Val(2p)	1.03466	-0.04147
412	C	22	pz	Ryd(3p)	0.00365	0.92297
413	C	22	pz	Ryd(4p)	0.00062	1.65553
414	C	22	dxy	Ryd(3d)	0.00054	2.35681
415	C	22	dxz	Ryd(3d)	0.00068	2.15133
416	C	22	dyz	Ryd(3d)	0.00072	2.46950
417	C	22	dx2y2	Ryd(3d)	0.00060	2.11023
418	C	22	dz2	Ryd(3d)	0.00081	2.55471
419	C	23	S	Cor(1S)	1.99909	-9.72332
420	C	23	S	Val(2S)	0.97332	-0.19771
421	C	23	S	Ryd(4S)	0.00104	1.40069
422	C	23	S	Ryd(3S)	0.00011	1.33878
423	C	23	S	Ryd(5S)	0.00000	21.29412
424	C	23	px	Val(2p)	1.01172	-0.08428
425	C	23	px	Ryd(3p)	0.00158	0.80871
426	C	23	px	Ryd(4p)	0.00052	1.21252
427	C	23	py	Val(2p)	1.04526	-0.05963
428	C	23	py	Ryd(3p)	0.00224	1.01377
429	C	23	py	Ryd(4p)	0.00040	1.29389
430	C	23	pz	Val(2p)	1.16588	-0.04797
431	C	23	pz	Ryd(4p)	0.00384	1.19624
432	C	23	pz	Ryd(3p)	0.00056	1.12107
433	C	23	dxy	Ryd(3d)	0.00054	2.37920
434	C	23	dxz	Ryd(3d)	0.00045	2.13006
435	C	23	dyz	Ryd(3d)	0.00071	2.40011
436	C	23	dx2y2	Ryd(3d)	0.00043	2.04986
437	C	23	dz2	Ryd(3d)	0.00065	2.52376
438	C	24	S	Cor(1S)	1.99920	-9.72885
439	C	24	S	Val(2S)	0.97700	-0.20429
440	C	24	S	Ryd(3S)	0.00081	1.06154
441	C	24	S	Ryd(4S)	0.00008	1.40826
442	C	24	S	Ryd(5S)	0.00000	21.18474
443	C	24	px	Val(2p)	1.03209	-0.08899
444	C	24	px	Ryd(3p)	0.00190	0.78444
445	C	24	px	Ryd(4p)	0.00032	1.28123
446	C	24	py	Val(2p)	1.07097	-0.06127
447	C	24	py	Ryd(3p)	0.00306	0.93377
448	C	24	py	Ryd(4p)	0.00033	1.31110
449	C	24	pz	Val(2p)	1.10083	-0.04643
450	C	24	pz	Ryd(3p)	0.00359	1.03122
451	C	24	pz	Ryd(4p)	0.00036	1.40022
452	C	24	dxy	Ryd(3d)	0.00052	2.33358
453	C	24	dxz	Ryd(3d)	0.00045	2.11146
454	C	24	dyz	Ryd(3d)	0.00065	2.40941
455	C	24	dx2y2	Ryd(3d)	0.00037	2.01261

456	C	24	dz2	Ryd(3d)	0.00082	2.52735
457	C	25	S	Cor(1S)	1.99909	-9.72677
458	C	25	S	Val(2S)	0.97228	-0.20182
459	C	25	S	Ryd(4S)	0.00095	1.40740
460	C	25	S	Ryd(3S)	0.00009	1.37567
461	C	25	S	Ryd(5S)	0.00000	21.26183
462	C	25	px	Val(2p)	1.05229	-0.09064
463	C	25	px	Ryd(3p)	0.00194	0.81739
464	C	25	px	Ryd(4p)	0.00056	1.15943
465	C	25	py	Val(2p)	1.12391	-0.06603
466	C	25	py	Ryd(3p)	0.00308	1.06448
467	C	25	py	Ryd(4p)	0.00050	1.16004
468	C	25	pz	Val(2p)	1.06008	-0.04882
469	C	25	pz	Ryd(3p)	0.00248	1.10684
470	C	25	pz	Ryd(4p)	0.00023	1.40356
471	C	25	dxy	Ryd(3d)	0.00048	2.32776
472	C	25	dxz	Ryd(3d)	0.00052	2.15430
473	C	25	dyz	Ryd(3d)	0.00072	2.41203
474	C	25	dx2y2	Ryd(3d)	0.00036	1.99865
475	C	25	dz2	Ryd(3d)	0.00068	2.57914
476	C	26	S	Cor(1S)	1.99898	-9.73994
477	C	26	S	Val(2S)	0.92193	-0.19298
478	C	26	S	Ryd(3S)	0.00168	0.96538
479	C	26	S	Ryd(4S)	0.00044	1.97754
480	C	26	S	Ryd(5S)	0.00000	21.18931
481	C	26	px	Val(2p)	1.00072	-0.08746
482	C	26	px	Ryd(3p)	0.00291	0.77586
483	C	26	px	Ryd(4p)	0.00027	1.45872
484	C	26	py	Val(2p)	1.02484	-0.06358
485	C	26	py	Ryd(3p)	0.00333	0.95374
486	C	26	py	Ryd(4p)	0.00047	1.55877
487	C	26	pz	Val(2p)	1.03289	-0.04442
488	C	26	pz	Ryd(3p)	0.00427	1.24672
489	C	26	pz	Ryd(4p)	0.00034	1.63913
490	C	26	dxy	Ryd(3d)	0.00061	2.40730
491	C	26	dxz	Ryd(3d)	0.00070	2.18238
492	C	26	dyz	Ryd(3d)	0.00075	2.47050
493	C	26	dx2y2	Ryd(3d)	0.00059	2.05581
494	C	26	dz2	Ryd(3d)	0.00067	2.46060
495	C	27	S	Cor(1S)	1.99936	-9.74225
496	C	27	S	Val(2S)	0.99682	-0.24649
497	C	27	S	Ryd(3S)	0.00147	1.18250
498	C	27	S	Ryd(4S)	0.00031	2.05089
499	C	27	S	Ryd(5S)	0.00001	20.97416
500	C	27	px	Val(2p)	1.10685	-0.07911
501	C	27	px	Ryd(3p)	0.00179	0.83743
502	C	27	px	Ryd(4p)	0.00036	1.43637
503	C	27	py	Val(2p)	1.02677	-0.07600
504	C	27	py	Ryd(3p)	0.00164	0.79534
505	C	27	py	Ryd(4p)	0.00053	1.42394
506	C	27	pz	Val(2p)	1.10935	-0.08034
507	C	27	pz	Ryd(3p)	0.00276	1.00954
508	C	27	pz	Ryd(4p)	0.00038	1.47703
509	C	27	dxy	Ryd(3d)	0.00082	2.49907
510	C	27	dxz	Ryd(3d)	0.00094	2.49227
511	C	27	dyz	Ryd(3d)	0.00051	2.23162
512	C	27	dx2y2	Ryd(3d)	0.00062	2.22601
513	C	27	dz2	Ryd(3d)	0.00066	2.41215
514	C	28	S	Cor(1S)	1.99941	-9.72951
515	C	28	S	Val(2S)	1.11723	-0.27656
516	C	28	S	Ryd(3S)	0.00058	1.19713
517	C	28	S	Ryd(4S)	0.00016	2.43073
518	C	28	S	Ryd(5S)	0.00000	20.59618
519	C	28	px	Val(2p)	1.15205	-0.08329
520	C	28	px	Ryd(3p)	0.00060	0.55276
521	C	28	px	Ryd(4p)	0.00032	1.52696
522	C	28	py	Val(2p)	1.12394	-0.08677

523	C	28	py	Ryd(3p)	0.00055	0.55910
524	C	28	py	Ryd(4p)	0.00048	1.47266
525	C	28	pz	Val(2p)	1.21451	-0.08399
526	C	28	pz	Ryd(3p)	0.00107	0.54223
527	C	28	pz	Ryd(4p)	0.00006	1.50317
528	C	28	dxy	Ryd(3d)	0.00064	2.47876
529	C	28	dxz	Ryd(3d)	0.00074	2.44375
530	C	28	dyz	Ryd(3d)	0.00025	2.15267
531	C	28	dx2y2	Ryd(3d)	0.00053	2.23459
532	C	28	dz2	Ryd(3d)	0.00055	2.38674
533	C	29	S	Cor(1S)	1.99937	-9.75206
534	C	29	S	Val(2S)	0.99666	-0.25611
535	C	29	S	Ryd(4S)	0.00118	1.71925
536	C	29	S	Ryd(3S)	0.00005	1.64589
537	C	29	S	Ryd(5S)	0.00000	21.20778
538	C	29	px	Val(2p)	1.06603	-0.08945
539	C	29	px	Ryd(3p)	0.00178	0.95523
540	C	29	px	Ryd(4p)	0.00039	1.42277
541	C	29	py	Val(2p)	1.10882	-0.09020
542	C	29	py	Ryd(3p)	0.00240	1.02511
543	C	29	py	Ryd(4p)	0.00029	1.35859
544	C	29	pz	Val(2p)	1.06596	-0.08593
545	C	29	pz	Ryd(3p)	0.00153	0.85610
546	C	29	pz	Ryd(4p)	0.00043	1.28745
547	C	29	dxy	Ryd(3d)	0.00071	2.36723
548	C	29	dxz	Ryd(3d)	0.00062	2.22988
549	C	29	dyz	Ryd(3d)	0.00077	2.34713
550	C	29	dx2y2	Ryd(3d)	0.00062	2.31506
551	C	29	dz2	Ryd(3d)	0.00078	2.51690
552	C	30	S	Cor(1S)	1.99942	-9.73526
553	C	30	S	Val(2S)	1.11595	-0.28296
554	C	30	S	Ryd(3S)	0.00058	1.05897
555	C	30	S	Ryd(4S)	0.00013	2.70815
556	C	30	S	Ryd(5S)	0.00000	20.32400
557	C	30	px	Val(2p)	1.07853	-0.09009
558	C	30	px	Ryd(3p)	0.00051	0.49738
559	C	30	px	Ryd(4p)	0.00055	1.44621
560	C	30	py	Val(2p)	1.21864	-0.09112
561	C	30	py	Ryd(3p)	0.00122	0.54366
562	C	30	py	Ryd(4p)	0.00004	1.48711
563	C	30	pz	Val(2p)	1.19711	-0.09233
564	C	30	pz	Ryd(3p)	0.00085	0.57101
565	C	30	pz	Ryd(4p)	0.00019	1.53517
566	C	30	dxy	Ryd(3d)	0.00076	2.38533
567	C	30	dxz	Ryd(3d)	0.00044	2.24749
568	C	30	dyz	Ryd(3d)	0.00027	2.21938
569	C	30	dx2y2	Ryd(3d)	0.00047	2.32363
570	C	30	dz2	Ryd(3d)	0.00071	2.46056
571	C	31	S	Cor(1S)	1.99874	-9.78499
572	C	31	S	Val(2S)	0.86698	-0.18374
573	C	31	S	Ryd(3S)	0.00118	0.96312
574	C	31	S	Ryd(4S)	0.00067	1.83273
575	C	31	S	Ryd(5S)	0.00000	21.56138
576	C	31	px	Val(2p)	0.93627	-0.07394
577	C	31	px	Ryd(3p)	0.00435	1.02588
578	C	31	px	Ryd(4p)	0.00071	1.67581
579	C	31	py	Val(2p)	1.06601	-0.09663
580	C	31	py	Ryd(3p)	0.00304	0.74573
581	C	31	py	Ryd(4p)	0.00043	1.61968
582	C	31	pz	Val(2p)	0.99331	-0.07441
583	C	31	pz	Ryd(3p)	0.00401	0.94722
584	C	31	pz	Ryd(4p)	0.00062	1.67278
585	C	31	dxy	Ryd(3d)	0.00067	2.45194
586	C	31	dxz	Ryd(3d)	0.00093	2.47741
587	C	31	dyz	Ryd(3d)	0.00071	2.41789
588	C	31	dx2y2	Ryd(3d)	0.00069	2.18296
589	C	31	dz2	Ryd(3d)	0.00077	2.33110

590	C	32	S	Cor(1S)	1.99898	-9.74810
591	C	32	S	Val(2S)	0.92384	-0.20127
592	C	32	S	Ryd(3S)	0.00167	0.91634
593	C	32	S	Ryd(4S)	0.00046	1.92102
594	C	32	S	Ryd(5S)	0.00000	21.08749
595	C	32	px	Val(2p)	1.02499	-0.06910
596	C	32	px	Ryd(3p)	0.00302	1.01211
597	C	32	px	Ryd(4p)	0.00040	1.48412
598	C	32	py	Val(2p)	0.99497	-0.08233
599	C	32	py	Ryd(3p)	0.00395	0.96976
600	C	32	py	Ryd(4p)	0.00026	1.47739
601	C	32	pz	Val(2p)	1.02810	-0.06469
602	C	32	pz	Ryd(3p)	0.00329	0.95864
603	C	32	pz	Ryd(4p)	0.00043	1.52051
604	C	32	dxy	Ryd(3d)	0.00052	2.33017
605	C	32	dxz	Ryd(3d)	0.00074	2.40795
606	C	32	dyz	Ryd(3d)	0.00063	2.40188
607	C	32	dx2y2	Ryd(3d)	0.00068	2.11757
608	C	32	dz2	Ryd(3d)	0.00074	2.27647
609	C	33	S	Cor(1S)	1.99910	-9.73591
610	C	33	S	Val(2S)	0.97357	-0.21131
611	C	33	S	Ryd(3S)	0.00097	1.38310
612	C	33	S	Ryd(4S)	0.00009	1.41500
613	C	33	S	Ryd(5S)	0.00000	21.22051
614	C	33	px	Val(2p)	1.03872	-0.07369
615	C	33	px	Ryd(3p)	0.00200	0.91960
616	C	33	px	Ryd(4p)	0.00041	1.27637
617	C	33	py	Val(2p)	1.05948	-0.08727
618	C	33	py	Ryd(3p)	0.00214	0.94620
619	C	33	py	Ryd(4p)	0.00046	1.28409
620	C	33	pz	Val(2p)	1.13523	-0.07099
621	C	33	pz	Ryd(3p)	0.00334	1.08613
622	C	33	pz	Ryd(4p)	0.00053	1.13493
623	C	33	dxy	Ryd(3d)	0.00058	2.39697
624	C	33	dxz	Ryd(3d)	0.00062	2.41235
625	C	33	dyz	Ryd(3d)	0.00057	2.26744
626	C	33	dx2y2	Ryd(3d)	0.00050	2.08573
627	C	33	dz2	Ryd(3d)	0.00051	2.25431
628	C	34	S	Cor(1S)	1.99920	-9.73939
629	C	34	S	Val(2S)	0.97772	-0.21491
630	C	34	S	Ryd(3S)	0.00082	1.05448
631	C	34	S	Ryd(4S)	0.00009	1.51899
632	C	34	S	Ryd(5S)	0.00000	21.16532
633	C	34	px	Val(2p)	1.10319	-0.07500
634	C	34	px	Ryd(3p)	0.00324	1.00133
635	C	34	px	Ryd(4p)	0.00025	1.54675
636	C	34	py	Val(2p)	1.02219	-0.08488
637	C	34	py	Ryd(3p)	0.00220	0.80375
638	C	34	py	Ryd(4p)	0.00024	1.16134
639	C	34	pz	Val(2p)	1.08072	-0.06856
640	C	34	pz	Ryd(3p)	0.00323	0.94991
641	C	34	pz	Ryd(4p)	0.00036	1.34029
642	C	34	dxy	Ryd(3d)	0.00059	2.36671
643	C	34	dxz	Ryd(3d)	0.00057	2.34048
644	C	34	dyz	Ryd(3d)	0.00060	2.34841
645	C	34	dx2y2	Ryd(3d)	0.00042	2.04093
646	C	34	dz2	Ryd(3d)	0.00064	2.24440
647	C	35	S	Cor(1S)	1.99909	-9.73496
648	C	35	S	Val(2S)	0.97404	-0.21028
649	C	35	S	Ryd(3S)	0.00098	1.40619
650	C	35	S	Ryd(4S)	0.00009	1.44430
651	C	35	S	Ryd(5S)	0.00000	21.26986
652	C	35	px	Val(2p)	1.09279	-0.07477
653	C	35	px	Ryd(3p)	0.00279	0.98350
654	C	35	px	Ryd(4p)	0.00038	1.21629
655	C	35	py	Val(2p)	1.09130	-0.08663
656	C	35	py	Ryd(3p)	0.00262	0.98917
657	C	35	py	Ryd(4p)	0.00043	1.24389

658	C	35	pz	Val(2p)	1.04813	-0.06716
659	C	35	pz	Ryd(3p)	0.00219	1.00746
660	C	35	pz	Ryd(4p)	0.00032	1.39364
661	C	35	dxy	Ryd(3d)	0.00056	2.34718
662	C	35	dxz	Ryd(3d)	0.00067	2.40867
663	C	35	dyz	Ryd(3d)	0.00057	2.32347
664	C	35	dx2y2	Ryd(3d)	0.00041	2.05923
665	C	35	dz2	Ryd(3d)	0.00058	2.28590
666	C	36	S	Cor(1S)	1.99898	-9.74600
667	C	36	S	Val(2S)	0.92317	-0.19849
668	C	36	S	Ryd(3S)	0.00166	0.89962
669	C	36	S	Ryd(4S)	0.00046	1.93233
670	C	36	S	Ryd(5S)	0.00000	21.14677
671	C	36	px	Val(2p)	1.02297	-0.07009
672	C	36	px	Ryd(3p)	0.00274	0.90945
673	C	36	px	Ryd(4p)	0.00043	1.54107
674	C	36	py	Val(2p)	0.99698	-0.07820
675	C	36	py	Ryd(3p)	0.00366	0.92995
676	C	36	py	Ryd(4p)	0.00031	1.53216
677	C	36	pz	Val(2p)	1.02035	-0.06062
678	C	36	pz	Ryd(3p)	0.00404	1.13364
679	C	36	pz	Ryd(4p)	0.00030	1.53426
680	C	36	dxy	Ryd(3d)	0.00063	2.43532
681	C	36	dxz	Ryd(3d)	0.00085	2.41863
682	C	36	dyz	Ryd(3d)	0.00056	2.36572
683	C	36	dx2y2	Ryd(3d)	0.00065	2.09176
684	C	36	dz2	Ryd(3d)	0.00067	2.23569
685	C	37	S	Cor(1S)	1.99937	-9.75573
686	C	37	S	Val(2S)	0.99683	-0.26043
687	C	37	S	Ryd(4S)	0.00118	1.70859
688	C	37	S	Ryd(3S)	0.00006	1.57394
689	C	37	S	Ryd(5S)	0.00000	21.16555
690	C	37	px	Val(2p)	1.11426	-0.09275
691	C	37	px	Ryd(3p)	0.00214	0.88810
692	C	37	px	Ryd(4p)	0.00038	1.32289
693	C	37	py	Val(2p)	1.03655	-0.09163
694	C	37	py	Ryd(3p)	0.00112	0.89406
695	C	37	py	Ryd(4p)	0.00042	1.33184
696	C	37	pz	Val(2p)	1.09213	-0.09363
697	C	37	pz	Ryd(3p)	0.00234	1.04974
698	C	37	pz	Ryd(4p)	0.00034	1.43766
699	C	37	dxy	Ryd(3d)	0.00075	2.44324
700	C	37	dxz	Ryd(3d)	0.00095	2.48589
701	C	37	dyz	Ryd(3d)	0.00047	2.17499
702	C	37	dx2y2	Ryd(3d)	0.00068	2.25930
703	C	37	dz2	Ryd(3d)	0.00062	2.38633
704	C	38	S	Cor(1S)	1.99943	-9.73821
705	C	38	S	Val(2S)	1.11477	-0.28570
706	C	38	S	Ryd(3S)	0.00056	1.10431
707	C	38	S	Ryd(4S)	0.00012	2.69113
708	C	38	S	Ryd(5S)	0.00000	20.31072
709	C	38	px	Val(2p)	1.19793	-0.09728
710	C	38	px	Ryd(3p)	0.00082	0.52789
711	C	38	px	Ryd(4p)	0.00019	1.52250
712	C	38	py	Val(2p)	1.21569	-0.09314
713	C	38	py	Ryd(3p)	0.00146	0.57925
714	C	38	py	Ryd(4p)	0.00004	1.49823
715	C	38	pz	Val(2p)	1.08328	-0.09308
716	C	38	pz	Ryd(3p)	0.00039	0.48831
717	C	38	pz	Ryd(4p)	0.00052	1.45163
718	C	38	dxy	Ryd(3d)	0.00060	2.41100
719	C	38	dxz	Ryd(3d)	0.00079	2.44149
720	C	38	dyz	Ryd(3d)	0.00028	2.12275
721	C	38	dx2y2	Ryd(3d)	0.00031	2.23543
722	C	38	dz2	Ryd(3d)	0.00066	2.40025
723	C	39	S	Cor(1S)	1.99936	-9.75034
724	C	39	S	Val(2S)	0.99689	-0.25484

725	C	39	S	Ryd(4S)	0.00120	1.71446
726	C	39	S	Ryd(3S)	0.00006	1.65794
727	C	39	S	Ryd(5S)	0.00000	21.21182
728	C	39	px	Val(2p)	1.13377	-0.08945
729	C	39	px	Ryd(3p)	0.00280	0.98747
730	C	39	px	Ryd(4p)	0.00026	1.37338
731	C	39	py	Val(2p)	1.04734	-0.08697
732	C	39	py	Ryd(3p)	0.00156	0.97627
733	C	39	py	Ryd(4p)	0.00042	1.45775
734	C	39	pz	Val(2p)	1.06175	-0.08554
735	C	39	pz	Ryd(3p)	0.00139	0.86066
736	C	39	pz	Ryd(4p)	0.00048	1.29633
737	C	39	dxy	Ryd(3d)	0.00055	2.22916
738	C	39	dxz	Ryd(3d)	0.00077	2.47088
739	C	39	dyz	Ryd(3d)	0.00078	2.39566
740	C	39	dx2y2	Ryd(3d)	0.00073	2.42226
741	C	39	dz2	Ryd(3d)	0.00063	2.27165
742	C	40	S	Cor(1S)	1.99942	-9.73507
743	C	40	S	Val(2S)	1.11676	-0.28274
744	C	40	S	Ryd(3S)	0.00058	1.09141
745	C	40	S	Ryd(4S)	0.00013	2.62677
746	C	40	S	Ryd(5S)	0.00000	20.37731
747	C	40	px	Val(2p)	1.21154	-0.09154
748	C	40	px	Ryd(3p)	0.00103	0.52734
749	C	40	px	Ryd(4p)	0.00009	1.48544
750	C	40	py	Val(2p)	1.06606	-0.09064
751	C	40	py	Ryd(3p)	0.00037	0.50375
752	C	40	py	Ryd(4p)	0.00062	1.44537
753	C	40	pz	Val(2p)	1.21477	-0.08968
754	C	40	pz	Ryd(3p)	0.00099	0.56998
755	C	40	pz	Ryd(4p)	0.00009	1.53712
756	C	40	dxy	Ryd(3d)	0.00048	2.22888
757	C	40	dxz	Ryd(3d)	0.00058	2.41521
758	C	40	dyz	Ryd(3d)	0.00064	2.32092
759	C	40	dx2y2	Ryd(3d)	0.00062	2.41041
760	C	40	dz2	Ryd(3d)	0.00031	2.26524
761	C	41	S	Cor(1S)	1.99874	-9.77446
762	C	41	S	Val(2S)	0.86843	-0.17345
763	C	41	S	Ryd(3S)	0.00122	0.96604
764	C	41	S	Ryd(4S)	0.00066	1.89331
765	C	41	S	Ryd(5S)	0.00000	21.52802
766	C	41	px	Val(2p)	1.04871	-0.09375
767	C	41	px	Ryd(3p)	0.00347	0.78065
768	C	41	px	Ryd(4p)	0.00045	1.63167
769	C	41	py	Val(2p)	0.88299	-0.04944
770	C	41	py	Ryd(3p)	0.00486	1.15418
771	C	41	py	Ryd(4p)	0.00085	1.71252
772	C	41	pz	Val(2p)	1.06475	-0.06910
773	C	41	pz	Ryd(3p)	0.00269	0.80439
774	C	41	pz	Ryd(4p)	0.00045	1.65745
775	C	41	dxy	Ryd(3d)	0.00064	2.37627
776	C	41	dxz	Ryd(3d)	0.00069	2.37323
777	C	41	dyz	Ryd(3d)	0.00097	2.47483
778	C	41	dx2y2	Ryd(3d)	0.00067	2.36785
779	C	41	dz2	Ryd(3d)	0.00087	2.33538
780	C	42	S	Cor(1S)	1.99899	-9.73542
781	C	42	S	Val(2S)	0.92637	-0.18757
782	C	42	S	Ryd(3S)	0.00157	0.92565
783	C	42	S	Ryd(4S)	0.00042	2.00385
784	C	42	S	Ryd(5S)	0.00000	21.18354
785	C	42	px	Val(2p)	0.98361	-0.07637
786	C	42	px	Ryd(3p)	0.00287	0.86919
787	C	42	px	Ryd(4p)	0.00022	1.42247
788	C	42	py	Val(2p)	1.03376	-0.04839
789	C	42	py	Ryd(3p)	0.00309	0.98801
790	C	42	py	Ryd(4p)	0.00049	1.61770
791	C	42	pz	Val(2p)	1.01656	-0.04834
792	C	42	pz	Ryd(3p)	0.00402	1.05397

793	C	42	pz	Ryd(4p)	0.00048	1.54207
794	C	42	dxy	Ryd(3d)	0.00063	2.30461
795	C	42	dxz	Ryd(3d)	0.00059	2.31531
796	C	42	dyz	Ryd(3d)	0.00076	2.43503
797	C	42	dx2y2	Ryd(3d)	0.00061	2.22109
798	C	42	dz2	Ryd(3d)	0.00076	2.35889
799	C	43	S	Cor(1S)	1.99910	-9.72422
800	C	43	S	Val(2S)	0.97460	-0.19998
801	C	43	S	Ryd(4S)	0.00095	1.38719
802	C	43	S	Ryd(3S)	0.00009	1.35718
803	C	43	S	Ryd(5S)	0.00000	21.29913
804	C	43	px	Val(2p)	1.03144	-0.08260
805	C	43	px	Ryd(3p)	0.00167	0.85705
806	C	43	px	Ryd(4p)	0.00046	1.25014
807	C	43	py	Val(2p)	1.06940	-0.05599
808	C	43	py	Ryd(3p)	0.00265	0.94334
809	C	43	py	Ryd(4p)	0.00052	1.21554
810	C	43	pz	Val(2p)	1.13491	-0.05907
811	C	43	pz	Ryd(3p)	0.00340	1.16033
812	C	43	pz	Ryd(4p)	0.00045	1.21641
813	C	43	dxy	Ryd(3d)	0.00057	2.32479
814	C	43	dxz	Ryd(3d)	0.00049	2.27323
815	C	43	dyz	Ryd(3d)	0.00062	2.45037
816	C	43	dx2y2	Ryd(3d)	0.00054	2.18782
817	C	43	dz2	Ryd(3d)	0.00054	2.24141
818	C	44	S	Cor(1S)	1.99919	-9.73043
819	C	44	S	Val(2S)	0.97697	-0.20579
820	C	44	S	Ryd(3S)	0.00078	1.03819
821	C	44	S	Ryd(4S)	0.00009	1.46269
822	C	44	S	Ryd(5S)	0.00000	21.17618
823	C	44	px	Val(2p)	1.02635	-0.08557
824	C	44	px	Ryd(3p)	0.00200	0.77998
825	C	44	px	Ryd(4p)	0.00030	1.22824
826	C	44	py	Val(2p)	1.13898	-0.05998
827	C	44	py	Ryd(3p)	0.00389	1.05373
828	C	44	py	Ryd(4p)	0.00039	1.63782
829	C	44	pz	Val(2p)	1.04297	-0.05741
830	C	44	pz	Ryd(3p)	0.00293	0.87832
831	C	44	pz	Ryd(4p)	0.00029	1.15787
832	C	44	dxy	Ryd(3d)	0.00046	2.25586
833	C	44	dxz	Ryd(3d)	0.00059	2.32161
834	C	44	dyz	Ryd(3d)	0.00073	2.41289
835	C	44	dx2y2	Ryd(3d)	0.00039	2.11101
836	C	44	dz2	Ryd(3d)	0.00064	2.27797
837	C	45	S	Cor(1S)	1.99909	-9.72713
838	C	45	S	Val(2S)	0.97249	-0.20254
839	C	45	S	Ryd(4S)	0.00097	1.39850
840	C	45	S	Ryd(3S)	0.00010	1.37146
841	C	45	S	Ryd(5S)	0.00000	21.24969
842	C	45	px	Val(2p)	1.07482	-0.08723
843	C	45	px	Ryd(3p)	0.00228	0.88105
844	C	45	px	Ryd(4p)	0.00061	1.19289
845	C	45	py	Val(2p)	1.07173	-0.05997
846	C	45	py	Ryd(3p)	0.00265	0.94295
847	C	45	py	Ryd(4p)	0.00049	1.18639
848	C	45	pz	Val(2p)	1.09377	-0.06133
849	C	45	pz	Ryd(3p)	0.00276	1.11724
850	C	45	pz	Ryd(4p)	0.00032	1.36592
851	C	45	dxy	Ryd(3d)	0.00055	2.30409
852	C	45	dxz	Ryd(3d)	0.00053	2.24942
853	C	45	dyz	Ryd(3d)	0.00064	2.46008
854	C	45	dx2y2	Ryd(3d)	0.00049	2.16994
855	C	45	dz2	Ryd(3d)	0.00055	2.27483
856	C	46	S	Cor(1S)	1.99898	-9.73862
857	C	46	S	Val(2S)	0.92411	-0.19225
858	C	46	S	Ryd(3S)	0.00168	0.92561
859	C	46	S	Ryd(4S)	0.00045	1.95497

860	C	46	S	Ryd(5S)	0.00000	21.15552
861	C	46	px	Val(2p)	1.00147	-0.08158
862	C	46	px	Ryd(3p)	0.00315	0.83146
863	C	46	px	Ryd(4p)	0.00029	1.48471
864	C	46	py	Val(2p)	1.03733	-0.05525
865	C	46	py	Ryd(3p)	0.00277	0.98313
866	C	46	py	Ryd(4p)	0.00044	1.53253
867	C	46	pz	Val(2p)	1.01373	-0.05341
868	C	46	pz	Ryd(3p)	0.00460	1.14572
869	C	46	pz	Ryd(4p)	0.00033	1.58237
870	C	46	dxy	Ryd(3d)	0.00058	2.31783
871	C	46	dxz	Ryd(3d)	0.00064	2.39191
872	C	46	dyz	Ryd(3d)	0.00076	2.40530
873	C	46	dx2y2	Ryd(3d)	0.00063	2.18208
874	C	46	dz2	Ryd(3d)	0.00071	2.27726
875	C	47	S	Cor(1S)	1.99935	-9.73178
876	C	47	S	Val(2S)	0.99796	-0.23625
877	C	47	S	Ryd(3S)	0.00123	1.28825
878	C	47	S	Ryd(4S)	0.00025	2.16423
879	C	47	S	Ryd(5S)	0.00001	20.81049
880	C	47	px	Val(2p)	1.08597	-0.06987
881	C	47	px	Ryd(3p)	0.00171	0.81683
882	C	47	px	Ryd(4p)	0.00046	1.53052
883	C	47	py	Val(2p)	1.09913	-0.07077
884	C	47	py	Ryd(3p)	0.00277	0.83818
885	C	47	py	Ryd(4p)	0.00055	1.53007
886	C	47	pz	Val(2p)	1.07483	-0.07041
887	C	47	pz	Ryd(3p)	0.00201	0.89556
888	C	47	pz	Ryd(4p)	0.00034	1.49744
889	C	47	dxy	Ryd(3d)	0.00090	2.55930
890	C	47	dxz	Ryd(3d)	0.00095	2.59783
891	C	47	dyz	Ryd(3d)	0.00094	2.56479
892	C	47	dx2y2	Ryd(3d)	0.00037	2.05846
893	C	47	dz2	Ryd(3d)	0.00034	2.13083
894	C	48	S	Cor(1S)	1.99941	-9.72114
895	C	48	S	Val(2S)	1.11731	-0.26757
896	C	48	S	Ryd(3S)	0.00060	1.20273
897	C	48	S	Ryd(4S)	0.00018	2.48676
898	C	48	S	Ryd(5S)	0.00000	20.56879
899	C	48	px	Val(2p)	1.16986	-0.07427
900	C	48	px	Ryd(3p)	0.00074	0.57852
901	C	48	px	Ryd(4p)	0.00023	1.55312
902	C	48	py	Val(2p)	1.16751	-0.07728
903	C	48	py	Ryd(3p)	0.00085	0.57206
904	C	48	py	Ryd(4p)	0.00029	1.49942
905	C	48	pz	Val(2p)	1.15218	-0.07657
906	C	48	pz	Ryd(3p)	0.00064	0.52536
907	C	48	pz	Ryd(4p)	0.00032	1.49306
908	C	48	dxy	Ryd(3d)	0.00079	2.52410
909	C	48	dxz	Ryd(3d)	0.00080	2.52346
910	C	48	dyz	Ryd(3d)	0.00080	2.49584
911	C	48	dx2y2	Ryd(3d)	0.00014	2.08995
912	C	48	dz2	Ryd(3d)	0.00020	2.10733
913	C	49	S	Cor(1S)	1.99937	-9.74876
914	C	49	S	Val(2S)	0.99642	-0.25314
915	C	49	S	Ryd(4S)	0.00119	1.72400
916	C	49	S	Ryd(3S)	0.00005	1.70258
917	C	49	S	Ryd(5S)	0.00000	21.21593
918	C	49	px	Val(2p)	1.06146	-0.08674
919	C	49	px	Ryd(3p)	0.00185	0.95158
920	C	49	px	Ryd(4p)	0.00042	1.42943
921	C	49	py	Val(2p)	1.15137	-0.08780
922	C	49	py	Ryd(3p)	0.00299	0.94354
923	C	49	py	Ryd(4p)	0.00029	1.36062
924	C	49	pz	Val(2p)	1.03217	-0.08423
925	C	49	pz	Ryd(3p)	0.00115	0.89450
926	C	49	pz	Ryd(4p)	0.00049	1.33938
927	C	49	dxy	Ryd(3d)	0.00071	2.32475

928	C	49	dxz	Ryd(3d)	0.00055	2.20260
929	C	49	dyz	Ryd(3d)	0.00064	2.43416
930	C	49	dx2y2	Ryd(3d)	0.00066	2.36549
931	C	49	dz2	Ryd(3d)	0.00094	2.45735
932	C	50	S	Cor(1S)	1.99942	-9.73331
933	C	50	S	Val(2S)	1.11610	-0.28088
934	C	50	S	Ryd(3S)	0.00060	1.02795
935	C	50	S	Ryd(4S)	0.00014	2.68109
936	C	50	S	Ryd(5S)	0.00000	20.38211
937	C	50	px	Val(2p)	1.06153	-0.08844
938	C	50	px	Ryd(3p)	0.00039	0.49390
939	C	50	px	Ryd(4p)	0.00063	1.44952
940	C	50	py	Val(2p)	1.21303	-0.09060
941	C	50	py	Ryd(3p)	0.00094	0.52986
942	C	50	py	Ryd(4p)	0.00012	1.51130
943	C	50	pz	Val(2p)	1.21897	-0.08794
944	C	50	pz	Ryd(3p)	0.00125	0.58966
945	C	50	pz	Ryd(4p)	0.00004	1.52441
946	C	50	dxy	Ryd(3d)	0.00068	2.34181
947	C	50	dxz	Ryd(3d)	0.00041	2.17383
948	C	50	dyz	Ryd(3d)	0.00056	2.41185
949	C	50	dx2y2	Ryd(3d)	0.00047	2.34147
950	C	50	dz2	Ryd(3d)	0.00052	2.38171
951	C	51	S	Cor(1S)	1.99937	-9.74918
952	C	51	S	Val(2S)	0.99674	-0.25373
953	C	51	S	Ryd(4S)	0.00117	1.73553
954	C	51	S	Ryd(3S)	0.00006	1.57332
955	C	51	S	Ryd(5S)	0.00000	21.16299
956	C	51	px	Val(2p)	1.06139	-0.08497
957	C	51	px	Ryd(3p)	0.00157	0.85849
958	C	51	px	Ryd(4p)	0.00041	1.35384
959	C	51	py	Val(2p)	1.07414	-0.08694
960	C	51	py	Ryd(3p)	0.00190	0.90903
961	C	51	py	Ryd(4p)	0.00041	1.41113
962	C	51	pz	Val(2p)	1.10859	-0.08750
963	C	51	pz	Ryd(3p)	0.00248	1.04285
964	C	51	pz	Ryd(4p)	0.00028	1.36614
965	C	51	dxy	Ryd(3d)	0.00081	2.46253
966	C	51	dxz	Ryd(3d)	0.00083	2.44346
967	C	51	dyz	Ryd(3d)	0.00090	2.50885
968	C	51	dx2y2	Ryd(3d)	0.00052	2.14114
969	C	51	dz2	Ryd(3d)	0.00042	2.21640
970	C	52	S	Cor(1S)	1.99942	-9.73327
971	C	52	S	Val(2S)	1.11615	-0.28084
972	C	52	S	Ryd(3S)	0.00057	1.06296
973	C	52	S	Ryd(4S)	0.00014	2.73358
974	C	52	S	Ryd(5S)	0.00000	20.31784
975	C	52	px	Val(2p)	1.15435	-0.09140
976	C	52	px	Ryd(3p)	0.00072	0.54051
977	C	52	px	Ryd(4p)	0.00034	1.51293
978	C	52	py	Val(2p)	1.13614	-0.08725
979	C	52	py	Ryd(3p)	0.00080	0.52547
980	C	52	py	Ryd(4p)	0.00035	1.47892
981	C	52	pz	Val(2p)	1.20333	-0.08849
982	C	52	pz	Ryd(3p)	0.00111	0.54168
983	C	52	pz	Ryd(4p)	0.00008	1.50030
984	C	52	dxy	Ryd(3d)	0.00065	2.45172
985	C	52	dxz	Ryd(3d)	0.00050	2.31901
986	C	52	dyz	Ryd(3d)	0.00085	2.50911
987	C	52	dx2y2	Ryd(3d)	0.00037	2.17055
988	C	52	dz2	Ryd(3d)	0.00027	2.19288
989	C	53	S	Cor(1S)	1.99935	-9.73236
990	C	53	S	Val(2S)	0.99743	-0.23675
991	C	53	S	Ryd(3S)	0.00131	1.22161
992	C	53	S	Ryd(4S)	0.00027	2.16940
993	C	53	S	Ryd(5S)	0.00001	20.88206
994	C	53	px	Val(2p)	1.06632	-0.07189

995	C	53	px	Ryd(3p)	0.00232	0.93201
996	C	53	px	Ryd(4p)	0.00048	1.57881
997	C	53	py	Val(2p)	1.15979	-0.07242
998	C	53	py	Ryd(3p)	0.00250	0.87094
999	C	53	py	Ryd(4p)	0.00035	1.50671
1000	C	53	pz	Val(2p)	1.02817	-0.06705
1001	C	53	pz	Ryd(3p)	0.00150	0.75769
1002	C	53	pz	Ryd(4p)	0.00049	1.45272
1003	C	53	dxy	Ryd(3d)	0.00070	2.31075
1004	C	53	dxz	Ryd(3d)	0.00056	2.26310
1005	C	53	dyz	Ryd(3d)	0.00054	2.29526
1006	C	53	dx2y2	Ryd(3d)	0.00070	2.43751
1007	C	53	dz2	Ryd(3d)	0.00101	2.61180
1008	C	54	S	Cor(1S)	1.99941	-9.72189
1009	C	54	S	Val(2S)	1.11757	-0.26857
1010	C	54	S	Ryd(3S)	0.00059	1.19756
1011	C	54	S	Ryd(4S)	0.00017	2.45958
1012	C	54	S	Ryd(5S)	0.00000	20.56164
1013	C	54	px	Val(2p)	1.18130	-0.07600
1014	C	54	px	Ryd(3p)	0.00108	0.56392
1015	C	54	px	Ryd(4p)	0.00020	1.50487
1016	C	54	py	Val(2p)	1.13298	-0.07561
1017	C	54	py	Ryd(3p)	0.00042	0.52806
1018	C	54	py	Ryd(4p)	0.00036	1.49568
1019	C	54	pz	Val(2p)	1.17393	-0.07863
1020	C	54	pz	Ryd(3p)	0.00068	0.56538
1021	C	54	pz	Ryd(4p)	0.00028	1.51709
1022	C	54	dxy	Ryd(3d)	0.00039	2.27768
1023	C	54	dxz	Ryd(3d)	0.00023	2.18490
1024	C	54	dyz	Ryd(3d)	0.00037	2.29302
1025	C	54	dx2y2	Ryd(3d)	0.00084	2.47126
1026	C	54	dz2	Ryd(3d)	0.00088	2.50613
1027	C	55	S	Cor(1S)	1.99942	-9.72860
1028	C	55	S	Val(2S)	1.11695	-0.27747
1029	C	55	S	Ryd(3S)	0.00063	1.22245
1030	C	55	S	Ryd(4S)	0.00022	2.53328
1031	C	55	S	Ryd(5S)	0.00000	20.70752
1032	C	55	px	Val(2p)	1.19623	-0.08482
1033	C	55	px	Ryd(3p)	0.00093	0.73525
1034	C	55	px	Ryd(4p)	0.00023	1.82287
1035	C	55	py	Val(2p)	1.06498	-0.08560
1036	C	55	py	Ryd(3p)	0.00076	0.63873
1037	C	55	py	Ryd(4p)	0.00053	1.63620
1038	C	55	pz	Val(2p)	1.23742	-0.08491
1039	C	55	pz	Ryd(3p)	0.00120	0.64074
1040	C	55	pz	Ryd(4p)	0.00033	1.56284
1041	C	55	dxy	Ryd(3d)	0.00067	2.42221
1042	C	55	dxz	Ryd(3d)	0.00063	2.43922
1043	C	55	dyz	Ryd(3d)	0.00034	2.15147
1044	C	55	dx2y2	Ryd(3d)	0.00043	2.29698
1045	C	55	dz2	Ryd(3d)	0.00059	2.41849
1046	C	56	S	Cor(1S)	1.99942	-9.72106
1047	C	56	S	Val(2S)	1.11491	-0.26989
1048	C	56	S	Ryd(3S)	0.00073	1.18856
1049	C	56	S	Ryd(4S)	0.00023	2.48012
1050	C	56	S	Ryd(5S)	0.00000	20.79066
1051	C	56	px	Val(2p)	1.10122	-0.07528
1052	C	56	px	Ryd(3p)	0.00069	0.68267
1053	C	56	px	Ryd(4p)	0.00039	1.76757
1054	C	56	py	Val(2p)	1.24202	-0.07714
1055	C	56	py	Ryd(3p)	0.00143	0.69604
1056	C	56	py	Ryd(4p)	0.00039	1.51333
1057	C	56	pz	Val(2p)	1.15616	-0.08042
1058	C	56	pz	Ryd(3p)	0.00100	0.72291
1059	C	56	pz	Ryd(4p)	0.00030	1.79215
1060	C	56	dxy	Ryd(3d)	0.00040	2.24039
1061	C	56	dxz	Ryd(3d)	0.00058	2.44151
1062	C	56	dyz	Ryd(3d)	0.00047	2.32368

1063	C	56	dx2y2	Ryd(3d)	0.00073	2.46588
1064	C	56	dz2	Ryd(3d)	0.00047	2.29475
1065	C	57	S	Cor(1S)	1.99943	-9.71209
1066	C	57	S	Val(2S)	1.11233	-0.25878
1067	C	57	S	Ryd(3S)	0.00068	1.27507
1068	C	57	S	Ryd(4S)	0.00021	2.56266
1069	C	57	S	Ryd(5S)	0.00000	20.61201
1070	C	57	px	Val(2p)	1.16213	-0.07069
1071	C	57	px	Ryd(3p)	0.00115	0.69975
1072	C	57	px	Ryd(4p)	0.00041	1.70442
1073	C	57	py	Val(2p)	1.16346	-0.06822
1074	C	57	py	Ryd(3p)	0.00117	0.60679
1075	C	57	py	Ryd(4p)	0.00030	1.59624
1076	C	57	pz	Val(2p)	1.17612	-0.06734
1077	C	57	pz	Ryd(3p)	0.00126	0.58198
1078	C	57	pz	Ryd(4p)	0.00031	1.64538
1079	C	57	dxy	Ryd(3d)	0.00081	2.53934
1080	C	57	dxz	Ryd(3d)	0.00080	2.51715
1081	C	57	dyz	Ryd(3d)	0.00073	2.54327
1082	C	57	dx2y2	Ryd(3d)	0.00015	2.09349
1083	C	57	dz2	Ryd(3d)	0.00016	2.10173
1084	C	58	S	Cor(1S)	1.99942	-9.72722
1085	C	58	S	Val(2S)	1.11473	-0.27525
1086	C	58	S	Ryd(3S)	0.00065	1.19038
1087	C	58	S	Ryd(4S)	0.00019	2.49299
1088	C	58	S	Ryd(5S)	0.00000	20.69911
1089	C	58	px	Val(2p)	1.22345	-0.08281
1090	C	58	px	Ryd(3p)	0.00122	0.66023
1091	C	58	px	Ryd(4p)	0.00031	1.49149
1092	C	58	py	Val(2p)	1.16202	-0.08269
1093	C	58	py	Ryd(3p)	0.00076	0.63623
1094	C	58	py	Ryd(4p)	0.00029	1.73070
1095	C	58	pz	Val(2p)	1.11292	-0.08497
1096	C	58	pz	Ryd(3p)	0.00086	0.62465
1097	C	58	pz	Ryd(4p)	0.00044	1.66909
1098	C	58	dxy	Ryd(3d)	0.00043	2.29344
1099	C	58	dxz	Ryd(3d)	0.00028	2.16527
1100	C	58	dyz	Ryd(3d)	0.00054	2.41180
1101	C	58	dx2y2	Ryd(3d)	0.00071	2.41813
1102	C	58	dz2	Ryd(3d)	0.00075	2.42434
1103	C	59	S	Cor(1S)	1.99942	-9.72792
1104	C	59	S	Val(2S)	1.11477	-0.27553
1105	C	59	S	Ryd(3S)	0.00061	1.11311
1106	C	59	S	Ryd(4S)	0.00016	2.76377
1107	C	59	S	Ryd(5S)	0.00000	20.47776
1108	C	59	px	Val(2p)	1.21304	-0.08398
1109	C	59	px	Ryd(3p)	0.00112	0.71435
1110	C	59	px	Ryd(4p)	0.00016	1.73909
1111	C	59	py	Val(2p)	1.16511	-0.08633
1112	C	59	py	Ryd(3p)	0.00107	0.59753
1113	C	59	py	Ryd(4p)	0.00029	1.58484
1114	C	59	pz	Val(2p)	1.12106	-0.08355
1115	C	59	pz	Ryd(3p)	0.00064	0.52734
1116	C	59	pz	Ryd(4p)	0.00042	1.60308
1117	C	59	dxy	Ryd(3d)	0.00069	2.43437
1118	C	59	dxz	Ryd(3d)	0.00059	2.38389
1119	C	59	dyz	Ryd(3d)	0.00068	2.48368
1120	C	59	dx2y2	Ryd(3d)	0.00026	2.19924
1121	C	59	dz2	Ryd(3d)	0.00041	2.21248
1122	C	60	S	Cor(1S)	1.99943	-9.70847
1123	C	60	S	Val(2S)	1.11166	-0.25536
1124	C	60	S	Ryd(3S)	0.00075	1.31412
1125	C	60	S	Ryd(4S)	0.00023	2.60024
1126	C	60	S	Ryd(5S)	0.00000	20.71304
1127	C	60	px	Val(2p)	1.06373	-0.06394
1128	C	60	px	Ryd(3p)	0.00065	0.67457
1129	C	60	px	Ryd(4p)	0.00056	1.55304

1130	C	60	py	Val(2p)	1.21219	-0.06346
1131	C	60	py	Ryd(3p)	0.00145	0.67952
1132	C	60	py	Ryd(4p)	0.00028	1.65929
1133	C	60	pz	Val(2p)	1.22631	-0.06766
1134	C	60	pz	Ryd(3p)	0.00144	0.67975
1135	C	60	pz	Ryd(4p)	0.00035	1.71386
1136	C	60	dxy	Ryd(3d)	0.00072	2.38262
1137	C	60	dxz	Ryd(3d)	0.00044	2.23568
1138	C	60	dyz	Ryd(3d)	0.00037	2.28519
1139	C	60	dx2y2	Ryd(3d)	0.00053	2.42118
1140	C	60	dz2	Ryd(3d)	0.00068	2.49798
1141	C	61	S	Cor(1S)	1.99942	-9.72639
1142	C	61	S	Val(2S)	1.11571	-0.27476
1143	C	61	S	Ryd(3S)	0.00065	1.24055
1144	C	61	S	Ryd(4S)	0.00019	2.54612
1145	C	61	S	Ryd(5S)	0.00000	20.70304
1146	C	61	px	Val(2p)	1.20165	-0.08292
1147	C	61	px	Ryd(3p)	0.00121	0.70571
1148	C	61	px	Ryd(4p)	0.00031	1.50078
1149	C	61	py	Val(2p)	1.08343	-0.08131
1150	C	61	py	Ryd(3p)	0.00060	0.57930
1151	C	61	py	Ryd(4p)	0.00052	1.66701
1152	C	61	pz	Val(2p)	1.21305	-0.08355
1153	C	61	pz	Ryd(3p)	0.00108	0.70110
1154	C	61	pz	Ryd(4p)	0.00022	1.77352
1155	C	61	dxy	Ryd(3d)	0.00054	2.35197
1156	C	61	dxz	Ryd(3d)	0.00028	2.20968
1157	C	61	dyz	Ryd(3d)	0.00047	2.29388
1158	C	61	dx2y2	Ryd(3d)	0.00072	2.39614
1159	C	61	dz2	Ryd(3d)	0.00065	2.47756
1160	C	62	S	Cor(1S)	1.99942	-9.71143
1161	C	62	S	Val(2S)	1.11380	-0.25999
1162	C	62	S	Ryd(3S)	0.00078	1.19177
1163	C	62	S	Ryd(4S)	0.00019	2.53795
1164	C	62	S	Ryd(5S)	0.00000	20.67893
1165	C	62	px	Val(2p)	1.19679	-0.07298
1166	C	62	px	Ryd(3p)	0.00116	0.66994
1167	C	62	px	Ryd(4p)	0.00028	1.68543
1168	C	62	py	Val(2p)	1.24406	-0.07072
1169	C	62	py	Ryd(3p)	0.00157	0.62826
1170	C	62	py	Ryd(4p)	0.00009	1.59873
1171	C	62	pz	Val(2p)	1.07167	-0.06793
1172	C	62	pz	Ryd(3p)	0.00050	0.55660
1173	C	62	pz	Ryd(4p)	0.00065	1.56910
1174	C	62	dxy	Ryd(3d)	0.00078	2.52987
1175	C	62	dxz	Ryd(3d)	0.00080	2.48686
1176	C	62	dyz	Ryd(3d)	0.00024	2.12734
1177	C	62	dx2y2	Ryd(3d)	0.00020	2.19994
1178	C	62	dz2	Ryd(3d)	0.00067	2.43543
1179	H	63	S	Val(1S)	0.75545	-0.00006
1180	H	63	S	Ryd(3S)	0.00043	1.79090
1181	H	63	S	Ryd(2S)	0.00009	0.80131
1182	H	63	px	Ryd(2p)	0.00055	2.72441
1183	H	63	py	Ryd(2p)	0.00020	1.83780
1184	H	63	pz	Ryd(2p)	0.00020	1.83821
1185	H	64	S	Val(1S)	0.75718	-0.00225
1186	H	64	S	Ryd(3S)	0.00043	1.76802
1187	H	64	S	Ryd(2S)	0.00009	0.77898
1188	H	64	px	Ryd(2p)	0.00013	1.96283
1189	H	64	py	Ryd(2p)	0.00042	2.21533
1190	H	64	pz	Ryd(2p)	0.00041	2.20575
1191	H	65	S	Val(1S)	0.78418	0.02546
1192	H	65	S	Ryd(2S)	0.00119	0.60573
1193	H	65	S	Ryd(3S)	0.00025	2.21725
1194	H	65	px	Ryd(2p)	0.00030	1.92371
1195	H	65	py	Ryd(2p)	0.00041	2.43311

1196	H	65	pz	Ryd(2p)	0.00016	2.08711
1197	H	66	S	Val(1S)	0.78213	0.02715
1198	H	66	S	Ryd(3S)	0.00029	1.21615
1199	H	66	S	Ryd(2S)	0.00018	1.14102
1200	H	66	px	Ryd(2p)	0.00026	1.89543
1201	H	66	py	Ryd(2p)	0.00025	2.15621
1202	H	66	pz	Ryd(2p)	0.00028	2.35279
1203	H	67	S	Val(1S)	0.77872	0.03448
1204	H	67	S	Ryd(2S)	0.00102	0.60382
1205	H	67	S	Ryd(3S)	0.00026	2.22154
1206	H	67	px	Ryd(2p)	0.00023	1.77975
1207	H	67	py	Ryd(2p)	0.00019	1.97766
1208	H	67	pz	Ryd(2p)	0.00046	2.70912
1209	H	68	S	Val(1S)	0.77961	0.02201
1210	H	68	S	Ryd(2S)	0.00134	0.60517
1211	H	68	S	Ryd(3S)	0.00028	2.24521
1212	H	68	px	Ryd(2p)	0.00033	2.25017
1213	H	68	py	Ryd(2p)	0.00036	2.19085
1214	H	68	pz	Ryd(2p)	0.00018	1.99399
1215	H	69	S	Val(1S)	0.78001	0.01924
1216	H	69	S	Ryd(2S)	0.00031	1.13532
1217	H	69	S	Ryd(3S)	0.00019	1.20200
1218	H	69	px	Ryd(2p)	0.00035	2.32887
1219	H	69	py	Ryd(2p)	0.00018	1.84901
1220	H	69	pz	Ryd(2p)	0.00027	2.20996
1221	H	70	S	Val(1S)	0.78187	0.01871
1222	H	70	S	Ryd(2S)	0.00113	0.59534
1223	H	70	S	Ryd(3S)	0.00025	2.20670
1224	H	70	px	Ryd(2p)	0.00019	1.92956
1225	H	70	py	Ryd(2p)	0.00026	1.98732
1226	H	70	pz	Ryd(2p)	0.00041	2.49692
1227	H	71	S	Val(1S)	0.75987	0.01397
1228	H	71	S	Ryd(3S)	0.00043	1.79046
1229	H	71	S	Ryd(2S)	0.00010	0.81350
1230	H	71	px	Ryd(2p)	0.00051	2.56812
1231	H	71	py	Ryd(2p)	0.00013	1.98132
1232	H	71	pz	Ryd(2p)	0.00037	1.90200
1233	H	72	S	Val(1S)	0.76024	0.01383
1234	H	72	S	Ryd(3S)	0.00044	1.76355
1235	H	72	S	Ryd(2S)	0.00010	0.82789
1236	H	72	px	Ryd(2p)	0.00018	2.00162
1237	H	72	py	Ryd(2p)	0.00054	2.71000
1238	H	72	pz	Ryd(2p)	0.00028	1.74205
1239	H	73	S	Val(1S)	0.78537	0.02432
1240	H	73	S	Ryd(2S)	0.00130	0.60137
1241	H	73	S	Ryd(3S)	0.00025	2.21321
1242	H	73	px	Ryd(2p)	0.00034	2.05381
1243	H	73	py	Ryd(2p)	0.00023	2.14663
1244	H	73	pz	Ryd(2p)	0.00029	2.23060
1245	H	74	S	Val(1S)	0.78298	0.02523
1246	H	74	S	Ryd(2S)	0.00032	1.16073
1247	H	74	S	Ryd(3S)	0.00019	1.18684
1248	H	74	px	Ryd(2p)	0.00023	1.86659
1249	H	74	py	Ryd(2p)	0.00040	2.54852
1250	H	74	pz	Ryd(2p)	0.00016	1.99016
1251	H	75	S	Val(1S)	0.77911	0.03410
1252	H	75	S	Ryd(2S)	0.00112	0.59965
1253	H	75	S	Ryd(3S)	0.00027	2.21782
1254	H	75	px	Ryd(2p)	0.00025	1.84584
1255	H	75	py	Ryd(2p)	0.00022	2.11747
1256	H	75	pz	Ryd(2p)	0.00040	2.49339

1257	H	76	S	Val(1S)	0.77901	0.03433
1258	H	76	S	Ryd(2S)	0.00127	0.61461
1259	H	76	S	Ryd(3S)	0.00028	2.24235
1260	H	76	px	Ryd(2p)	0.00039	2.35712
1261	H	76	py	Ryd(2p)	0.00028	1.96936
1262	H	76	pz	Ryd(2p)	0.00022	2.14611
1263	H	77	S	Val(1S)	0.78351	0.02500
1264	H	77	S	Ryd(2S)	0.00031	1.11544
1265	H	77	S	Ryd(3S)	0.00019	1.23573
1266	H	77	px	Ryd(2p)	0.00027	2.14814
1267	H	77	py	Ryd(2p)	0.00030	2.04146
1268	H	77	pz	Ryd(2p)	0.00022	2.20737
1269	H	78	S	Val(1S)	0.78550	0.02394
1270	H	78	S	Ryd(2S)	0.00124	0.60222
1271	H	78	S	Ryd(3S)	0.00024	2.21033
1272	H	78	px	Ryd(2p)	0.00019	1.94210
1273	H	78	py	Ryd(2p)	0.00022	1.82367
1274	H	78	pz	Ryd(2p)	0.00045	2.66211
1275	H	79	S	Val(1S)	0.77152	0.02881
1276	H	79	S	Ryd(2S)	0.00166	0.87202
1277	H	79	S	Ryd(3S)	0.00016	2.52594
1278	H	79	px	Ryd(2p)	0.00024	2.09640
1279	H	79	py	Ryd(2p)	0.00031	2.59878
1280	H	79	pz	Ryd(2p)	0.00021	2.02649
1281	H	80	S	Val(1S)	0.73341	0.07029
1282	H	80	S	Ryd(2S)	0.00353	0.77273
1283	H	80	S	Ryd(3S)	0.00024	2.54707
1284	H	80	px	Ryd(2p)	0.00033	2.32053
1285	H	80	py	Ryd(2p)	0.00020	2.26226
1286	H	80	pz	Ryd(2p)	0.00019	2.19215
1287	H	81	S	Val(1S)	0.77214	0.02743
1288	H	81	S	Ryd(2S)	0.00176	0.83518
1289	H	81	S	Ryd(3S)	0.00018	2.47282
1290	H	81	px	Ryd(2p)	0.00023	2.19652
1291	H	81	py	Ryd(2p)	0.00023	2.15904
1292	H	81	pz	Ryd(2p)	0.00035	2.34035
1293	H	82	S	Val(1S)	0.74296	0.06326
1294	H	82	S	Ryd(2S)	0.00299	0.74796
1295	H	82	S	Ryd(3S)	0.00022	2.49807
1296	H	82	px	Ryd(2p)	0.00017	2.09424
1297	H	82	py	Ryd(2p)	0.00038	2.61831
1298	H	82	pz	Ryd(2p)	0.00017	2.07432
1299	H	83	S	Val(1S)	0.78007	0.01976
1300	H	83	S	Ryd(2S)	0.00171	0.80962
1301	H	83	S	Ryd(3S)	0.00015	2.48728
1302	H	83	px	Ryd(2p)	0.00025	2.11268
1303	H	83	py	Ryd(2p)	0.00030	2.30492
1304	H	83	pz	Ryd(2p)	0.00023	2.29157
1305	H	84	S	Val(1S)	0.76670	0.03664
1306	H	84	S	Ryd(2S)	0.00174	0.71666
1307	H	84	S	Ryd(3S)	0.00019	2.48323
1308	H	84	px	Ryd(2p)	0.00031	2.41738
1309	H	84	py	Ryd(2p)	0.00015	2.01017
1310	H	84	pz	Ryd(2p)	0.00024	2.28875
1311	H	85	S	Val(1S)	0.77807	0.01579
1312	H	85	S	Ryd(2S)	0.00180	0.77717
1313	H	85	S	Ryd(3S)	0.00017	2.42371
1314	H	85	px	Ryd(2p)	0.00029	2.48581
1315	H	85	py	Ryd(2p)	0.00019	1.94487
1316	H	85	pz	Ryd(2p)	0.00031	2.25159

1317	H	86	S	Val(1S)	0.77367	0.02410
1318	H	86	S	Ryd(2S)	0.00158	0.73901
1319	H	86	S	Ryd(3S)	0.00016	2.38593
1320	H	86	px	Ryd(2p)	0.00029	2.41012
1321	H	86	py	Ryd(2p)	0.00024	2.04421
1322	H	86	pz	Ryd(2p)	0.00023	2.20233
1323	H	87	S	Val(1S)	0.78542	0.03308
1324	H	87	S	Ryd(2S)	0.00059	0.63094
1325	H	87	S	Ryd(3S)	0.00013	1.84773
1326	H	87	px	Ryd(2p)	0.00022	2.11263
1327	H	87	py	Ryd(2p)	0.00030	2.38837
1328	H	87	pz	Ryd(2p)	0.00013	1.86769
1329	H	88	S	Val(1S)	0.80078	0.02583
1330	H	88	S	Ryd(2S)	0.00068	0.91421
1331	H	88	S	Ryd(3S)	0.00018	1.57466
1332	H	88	px	Ryd(2p)	0.00027	2.20338
1333	H	88	py	Ryd(2p)	0.00016	1.83060
1334	H	88	pz	Ryd(2p)	0.00024	2.35812
1335	H	89	S	Val(1S)	0.73700	0.07509
1336	H	89	S	Ryd(2S)	0.00088	1.12983
1337	H	89	S	Ryd(3S)	0.00017	1.82789
1338	H	89	px	Ryd(2p)	0.00022	2.18818
1339	H	89	py	Ryd(2p)	0.00031	2.38465
1340	H	89	pz	Ryd(2p)	0.00014	1.88266
1341	H	90	S	Val(1S)	0.78364	0.02266
1342	H	90	S	Ryd(2S)	0.00060	0.67675
1343	H	90	S	Ryd(3S)	0.00013	1.74839
1344	H	90	px	Ryd(2p)	0.00020	1.97931
1345	H	90	py	Ryd(2p)	0.00025	2.47082
1346	H	90	pz	Ryd(2p)	0.00017	1.89307
1347	H	91	S	Val(1S)	0.79026	0.02240
1348	H	91	S	Ryd(2S)	0.00059	1.04313
1349	H	91	S	Ryd(3S)	0.00011	1.56359
1350	H	91	px	Ryd(2p)	0.00015	1.93978
1351	H	91	py	Ryd(2p)	0.00012	1.89231
1352	H	91	pz	Ryd(2p)	0.00035	2.53264
1353	H	92	S	Val(1S)	0.78793	0.02170
1354	H	92	S	Ryd(2S)	0.00085	0.78362
1355	H	92	S	Ryd(3S)	0.00012	1.64852
1356	H	92	px	Ryd(2p)	0.00026	2.36325
1357	H	92	py	Ryd(2p)	0.00013	1.84886
1358	H	92	pz	Ryd(2p)	0.00025	2.16247
1359	H	93	S	Val(1S)	0.78404	0.01628
1360	H	93	S	Ryd(2S)	0.00058	0.63777
1361	H	93	S	Ryd(3S)	0.00013	1.74520
1362	H	93	px	Ryd(2p)	0.00011	1.80572
1363	H	93	py	Ryd(2p)	0.00015	1.85179
1364	H	93	pz	Ryd(2p)	0.00037	2.65761
1365	H	94	S	Val(1S)	0.78819	0.01517
1366	H	94	S	Ryd(2S)	0.00073	0.91439
1367	H	94	S	Ryd(3S)	0.00015	1.54063
1368	H	94	px	Ryd(2p)	0.00017	2.11367
1369	H	94	py	Ryd(2p)	0.00027	2.20582
1370	H	94	pz	Ryd(2p)	0.00022	1.99877
1371	H	95	S	Val(1S)	0.78467	0.01728
1372	H	95	S	Ryd(2S)	0.00050	0.70989
1373	H	95	S	Ryd(3S)	0.00012	1.78401
1374	H	95	px	Ryd(2p)	0.00016	1.99726
1375	H	95	py	Ryd(2p)	0.00031	2.48400
1376	H	95	pz	Ryd(2p)	0.00014	1.82116
1377	H	96	S	Val(1S)	0.78602	0.02163

1378	H	96	S	Ryd(2S)	0.00074	0.58586
1379	H	96	S	Ryd(3S)	0.00015	1.89840
1380	H	96	px	Ryd(2p)	0.00016	1.83523
1381	H	96	py	Ryd(2p)	0.00013	1.90370
1382	H	96	pz	Ryd(2p)	0.00037	2.64065
1383	H	97	S	Val(1S)	0.75954	0.04748
1384	H	97	S	Ryd(2S)	0.00088	0.87543
1385	H	97	S	Ryd(3S)	0.00025	2.46614
1386	H	97	px	Ryd(2p)	0.00032	2.66180
1387	H	97	py	Ryd(2p)	0.00011	1.86284
1388	H	97	pz	Ryd(2p)	0.00015	1.92667
1389	H	98	S	Val(1S)	0.79127	0.02011
1390	H	98	S	Ryd(2S)	0.00069	0.97720
1391	H	98	S	Ryd(3S)	0.00017	1.53464
1392	H	98	px	Ryd(2p)	0.00021	2.00260
1393	H	98	py	Ryd(2p)	0.00024	2.34858
1394	H	98	pz	Ryd(2p)	0.00022	2.04004
1395	H	99	S	Val(1S)	0.78131	0.01844
1396	H	99	S	Ryd(2S)	0.00057	0.64335
1397	H	99	S	Ryd(3S)	0.00013	1.74132
1398	H	99	px	Ryd(2p)	0.00015	1.84027
1399	H	99	py	Ryd(2p)	0.00014	2.04721
1400	H	99	pz	Ryd(2p)	0.00034	2.43069
1401	H	100	S	Val(1S)	0.78971	0.01457
1402	H	100	S	Ryd(2S)	0.00076	0.86018
1403	H	100	S	Ryd(3S)	0.00014	1.59167
1404	H	100	px	Ryd(2p)	0.00030	2.27941
1405	H	100	py	Ryd(2p)	0.00015	2.03538
1406	H	100	pz	Ryd(2p)	0.00021	2.00625
1407	H	101	S	Val(1S)	0.78575	0.01727
1408	H	101	S	Ryd(2S)	0.00053	0.70800
1409	H	101	S	Ryd(3S)	0.00012	1.80274
1410	H	101	px	Ryd(2p)	0.00029	2.41507
1411	H	101	py	Ryd(2p)	0.00011	1.83527
1412	H	101	pz	Ryd(2p)	0.00021	2.05149
1413	H	102	S	Val(1S)	0.78209	0.02805
1414	H	102	S	Ryd(2S)	0.00056	0.64777
1415	H	102	S	Ryd(3S)	0.00015	1.82625
1416	H	102	px	Ryd(2p)	0.00016	1.86124
1417	H	102	py	Ryd(2p)	0.00020	2.03557
1418	H	102	pz	Ryd(2p)	0.00031	2.52869
1419	H	103	S	Val(1S)	0.75294	0.05728
1420	H	103	S	Ryd(2S)	0.00069	0.94945
1421	H	103	S	Ryd(3S)	0.00021	2.55374
1422	H	103	px	Ryd(2p)	0.00012	1.90447
1423	H	103	py	Ryd(2p)	0.00034	2.66727
1424	H	103	pz	Ryd(2p)	0.00012	1.90911
1425	H	104	S	Val(1S)	0.79353	0.02302
1426	H	104	S	Ryd(2S)	0.00073	0.90811
1427	H	104	S	Ryd(3S)	0.00019	1.69129
1428	H	104	px	Ryd(2p)	0.00030	2.44087
1429	H	104	py	Ryd(2p)	0.00018	1.97203
1430	H	104	pz	Ryd(2p)	0.00020	1.99216
1431	H	105	S	Val(1S)	0.78132	0.01442
1432	H	105	S	Ryd(2S)	0.00054	0.63731
1433	H	105	S	Ryd(3S)	0.00013	1.73549
1434	H	105	px	Ryd(2p)	0.00027	2.29258
1435	H	105	py	Ryd(2p)	0.00025	2.13967
1436	H	105	pz	Ryd(2p)	0.00011	1.85447
1437	H	106	S	Val(1S)	0.78269	0.01512
1438	H	106	S	Ryd(2S)	0.00049	0.63519

1439	H	106	S	Ryd(3S)	0.00013	1.80506
1440	H	106	px	Ryd(2p)	0.00017	1.94433
1441	H	106	py	Ryd(2p)	0.00033	2.52444
1442	H	106	pz	Ryd(2p)	0.00011	1.81555
1443	H	107	S	Val(1S)	0.79026	0.01060
1444	H	107	S	Ryd(2S)	0.00071	0.93365
1445	H	107	S	Ryd(3S)	0.00016	1.52577
1446	H	107	px	Ryd(2p)	0.00028	2.21165
1447	H	107	py	Ryd(2p)	0.00015	1.80850
1448	H	107	pz	Ryd(2p)	0.00023	2.25700
1449	H	108	S	Val(1S)	0.78460	0.02002
1450	H	108	S	Ryd(2S)	0.00073	0.60248
1451	H	108	S	Ryd(3S)	0.00015	1.89092
1452	H	108	px	Ryd(2p)	0.00028	2.23927
1453	H	108	py	Ryd(2p)	0.00022	2.24783
1454	H	108	pz	Ryd(2p)	0.00016	1.88556
1455	H	109	S	Val(1S)	0.79003	0.01860
1456	H	109	S	Ryd(2S)	0.00085	0.81596
1457	H	109	S	Ryd(3S)	0.00018	1.77591
1458	H	109	px	Ryd(2p)	0.00030	2.32844
1459	H	109	py	Ryd(2p)	0.00013	1.88698
1460	H	109	pz	Ryd(2p)	0.00024	2.18477
1461	H	110	S	Val(1S)	0.75556	0.04759
1462	H	110	S	Ryd(2S)	0.00064	0.88796
1463	H	110	S	Ryd(3S)	0.00022	2.52048
1464	H	110	px	Ryd(2p)	0.00018	1.95588
1465	H	110	py	Ryd(2p)	0.00010	1.93583
1466	H	110	pz	Ryd(2p)	0.00032	2.58610
1467	H	111	S	Val(1S)	0.78672	0.01961
1468	H	111	S	Ryd(2S)	0.00072	0.61995
1469	H	111	S	Ryd(3S)	0.00014	1.83966
1470	H	111	px	Ryd(2p)	0.00033	2.40056
1471	H	111	py	Ryd(2p)	0.00018	1.96340
1472	H	111	pz	Ryd(2p)	0.00017	1.98654
1473	H	112	S	Val(1S)	0.79290	0.01737
1474	H	112	S	Ryd(2S)	0.00082	0.83015
1475	H	112	S	Ryd(3S)	0.00017	1.69152
1476	H	112	px	Ryd(2p)	0.00023	2.05338
1477	H	112	py	Ryd(2p)	0.00020	2.00126
1478	H	112	pz	Ryd(2p)	0.00025	2.31990
1479	H	113	S	Val(1S)	0.76404	0.04192
1480	H	113	S	Ryd(2S)	0.00044	1.26053
1481	H	113	S	Ryd(3S)	0.00008	2.10641
1482	H	113	px	Ryd(2p)	0.00020	2.10158
1483	H	113	py	Ryd(2p)	0.00021	2.39888
1484	H	113	pz	Ryd(2p)	0.00016	1.92369
1485	H	114	S	Val(1S)	0.78418	0.01830
1486	H	114	S	Ryd(2S)	0.00059	0.63387
1487	H	114	S	Ryd(3S)	0.00014	1.75572
1488	H	114	px	Ryd(2p)	0.00029	2.46233
1489	H	114	py	Ryd(2p)	0.00018	1.91928
1490	H	114	pz	Ryd(2p)	0.00017	1.93262
1491	H	115	S	Val(1S)	0.78240	0.02111
1492	H	115	S	Ryd(2S)	0.00051	0.72657
1493	H	115	S	Ryd(3S)	0.00012	1.75991
1494	H	115	px	Ryd(2p)	0.00014	1.89622
1495	H	115	py	Ryd(2p)	0.00020	2.12270
1496	H	115	pz	Ryd(2p)	0.00026	2.29323
1497	H	116	S	Val(1S)	0.79000	0.01607
1498	H	116	S	Ryd(2S)	0.00075	0.89041
1499	H	116	S	Ryd(3S)	0.00015	1.56445

1500	H	116	px	Ryd(2p)	0.00019	1.95637
1501	H	116	py	Ryd(2p)	0.00020	2.10505
1502	H	116	pz	Ryd(2p)	0.00027	2.25089
1503	H	117	S	Val(1S)	0.78063	0.03275
1504	H	117	S	Ryd(2S)	0.00058	0.69359
1505	H	117	S	Ryd(3S)	0.00013	1.74461
1506	H	117	px	Ryd(2p)	0.00014	1.85025
1507	H	117	py	Ryd(2p)	0.00014	1.85559
1508	H	117	pz	Ryd(2p)	0.00032	2.66936
1509	H	118	S	Val(1S)	0.79236	0.02678
1510	H	118	S	Ryd(2S)	0.00084	0.77086
1511	H	118	S	Ryd(3S)	0.00012	1.67362
1512	H	118	px	Ryd(2p)	0.00018	1.92431
1513	H	118	py	Ryd(2p)	0.00032	2.59230
1514	H	118	pz	Ryd(2p)	0.00015	1.87000
1515	H	119	S	Val(1S)	0.78849	0.03136
1516	H	119	S	Ryd(2S)	0.00060	0.98558
1517	H	119	S	Ryd(3S)	0.00011	1.64427
1518	H	119	px	Ryd(2p)	0.00034	2.69236
1519	H	119	py	Ryd(2p)	0.00014	1.82501
1520	H	119	pz	Ryd(2p)	0.00014	1.86975
1521	H	120	S	Val(1S)	0.76926	0.05063
1522	H	120	S	Ryd(2S)	0.00053	0.74423
1523	H	120	S	Ryd(3S)	0.00014	1.72672
1524	H	120	px	Ryd(2p)	0.00011	1.85860
1525	H	120	py	Ryd(2p)	0.00018	1.92197
1526	H	120	pz	Ryd(2p)	0.00033	2.65841
1527	H	121	S	Val(1S)	0.76360	0.06167
1528	H	121	S	Ryd(2S)	0.00079	0.81272
1529	H	121	S	Ryd(3S)	0.00020	2.45714
1530	H	121	px	Ryd(2p)	0.00014	2.11109
1531	H	121	py	Ryd(2p)	0.00027	2.28320
1532	H	121	pz	Ryd(2p)	0.00016	2.10406
1533	H	122	S	Val(1S)	0.80520	0.02875
1534	H	122	S	Ryd(2S)	0.00070	0.83463
1535	H	122	S	Ryd(3S)	0.00020	1.66866
1536	H	122	px	Ryd(2p)	0.00017	2.07325
1537	H	122	py	Ryd(2p)	0.00035	2.49322
1538	H	122	pz	Ryd(2p)	0.00016	1.84886
1539	H	123	S	Val(1S)	0.76792	0.04954
1540	H	123	S	Ryd(2S)	0.00067	0.70450
1541	H	123	S	Ryd(3S)	0.00014	1.81082
1542	H	123	px	Ryd(2p)	0.00022	2.25531
1543	H	123	py	Ryd(2p)	0.00022	2.05784
1544	H	123	pz	Ryd(2p)	0.00018	2.09328
1545	H	124	S	Val(1S)	0.80245	0.02773
1546	H	124	S	Ryd(2S)	0.00070	0.86851
1547	H	124	S	Ryd(3S)	0.00018	1.62433
1548	H	124	px	Ryd(2p)	0.00021	2.03562
1549	H	124	py	Ryd(2p)	0.00020	2.12112
1550	H	124	pz	Ryd(2p)	0.00025	2.23639
1551	H	125	S	Val(1S)	0.77264	0.04769
1552	H	125	S	Ryd(2S)	0.00053	0.77061
1553	H	125	S	Ryd(3S)	0.00015	2.10057
1554	H	125	px	Ryd(2p)	0.00019	2.09747
1555	H	125	py	Ryd(2p)	0.00021	2.18799
1556	H	125	pz	Ryd(2p)	0.00021	2.14163
1557	H	126	S	Val(1S)	0.77990	0.03374
1558	H	126	S	Ryd(2S)	0.00057	0.69782
1559	H	126	S	Ryd(3S)	0.00013	1.74165
1560	H	126	px	Ryd(2p)	0.00024	2.10767

1561	H	126	py	Ryd(2p)	0.00017	2.06630
1562	H	126	pz	Ryd(2p)	0.00019	2.21072
1563	H	127	S	Val(1S)	0.78610	0.03408
1564	H	127	S	Ryd(2S)	0.00059	1.10145
1565	H	127	S	Ryd(3S)	0.00012	1.54770
1566	H	127	px	Ryd(2p)	0.00018	2.09043
1567	H	127	py	Ryd(2p)	0.00023	2.27263
1568	H	127	pz	Ryd(2p)	0.00022	2.05125
1569	H	128	S	Val(1S)	0.79321	0.02684
1570	H	128	S	Ryd(2S)	0.00084	0.75753
1571	H	128	S	Ryd(3S)	0.00012	1.68447
1572	H	128	px	Ryd(2p)	0.00022	2.18818
1573	H	128	py	Ryd(2p)	0.00024	2.08634
1574	H	128	pz	Ryd(2p)	0.00019	2.11489
1575	H	129	S	Val(1S)	0.78416	0.01812
1576	H	129	S	Ryd(2S)	0.00059	0.63319
1577	H	129	S	Ryd(3S)	0.00013	1.76183
1578	H	129	px	Ryd(2p)	0.00011	1.88672
1579	H	129	py	Ryd(2p)	0.00020	2.01831
1580	H	129	pz	Ryd(2p)	0.00032	2.41811
1581	H	130	S	Val(1S)	0.78995	0.01615
1582	H	130	S	Ryd(2S)	0.00076	0.87756
1583	H	130	S	Ryd(3S)	0.00015	1.57210
1584	H	130	px	Ryd(2p)	0.00016	2.10565
1585	H	130	py	Ryd(2p)	0.00034	2.40488
1586	H	130	pz	Ryd(2p)	0.00015	1.82022
1587	H	131	S	Val(1S)	0.78295	0.02104
1588	H	131	S	Ryd(2S)	0.00057	0.77435
1589	H	131	S	Ryd(3S)	0.00011	1.74234
1590	H	131	px	Ryd(2p)	0.00012	1.89364
1591	H	131	py	Ryd(2p)	0.00021	2.12270
1592	H	131	pz	Ryd(2p)	0.00026	2.29508
1593	H	132	S	Val(1S)	0.78564	0.02073
1594	H	132	S	Ryd(2S)	0.00073	0.56044
1595	H	132	S	Ryd(3S)	0.00016	1.91335
1596	H	132	px	Ryd(2p)	0.00017	1.87457
1597	H	132	py	Ryd(2p)	0.00021	1.98693
1598	H	132	pz	Ryd(2p)	0.00027	2.50432
1599	H	133	S	Val(1S)	0.76264	0.04502
1600	H	133	S	Ryd(2S)	0.00089	0.83922
1601	H	133	S	Ryd(3S)	0.00022	2.42096
1602	H	133	px	Ryd(2p)	0.00034	2.69790
1603	H	133	py	Ryd(2p)	0.00014	1.83706
1604	H	133	pz	Ryd(2p)	0.00012	1.86101
1605	H	134	S	Val(1S)	0.79518	0.01655
1606	H	134	S	Ryd(2S)	0.00072	0.91314
1607	H	134	S	Ryd(3S)	0.00018	1.57788
1608	H	134	px	Ryd(2p)	0.00020	1.99169
1609	H	134	py	Ryd(2p)	0.00034	2.52503
1610	H	134	pz	Ryd(2p)	0.00014	1.85737

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WARNING:  1 low occupancy (<1.9990e) core orbital  found on  C    1
          1 low occupancy (<1.9990e) core orbital  found on  C    3
          1 low occupancy (<1.9990e) core orbital  found on  C    4
          1 low occupancy (<1.9990e) core orbital  found on  C    5
          1 low occupancy (<1.9990e) core orbital  found on  C   10
          1 low occupancy (<1.9990e) core orbital  found on  B   14
          1 low occupancy (<1.9990e) core orbital  found on  B   15
          1 low occupancy (<1.9990e) core orbital  found on  C   16
          1 low occupancy (<1.9990e) core orbital  found on  C   21
          1 low occupancy (<1.9990e) core orbital  found on  C   22
          1 low occupancy (<1.9990e) core orbital  found on  C   26
          1 low occupancy (<1.9990e) core orbital  found on  C   31
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          1 low occupancy (<1.9990e) core orbital  found on  C   32
          1 low occupancy (<1.9990e) core orbital  found on  C   36
          1 low occupancy (<1.9990e) core orbital  found on  C   41
          1 low occupancy (<1.9990e) core orbital  found on  C   42
          1 low occupancy (<1.9990e) core orbital  found on  C   46

WARNING:  Population inversion found on atom  C    6
          Population inversion found on atom  C    8
          Population inversion found on atom  C   10
          Population inversion found on atom  B   14
          Population inversion found on atom  B   15
          Population inversion found on atom  C   16
          Population inversion found on atom  C   23
          Population inversion found on atom  C   25
          Population inversion found on atom  C   29
          Population inversion found on atom  C   30
          Population inversion found on atom  C   37
          Population inversion found on atom  C   38
          Population inversion found on atom  C   39
          Population inversion found on atom  C   40
          Population inversion found on atom  C   43
          Population inversion found on atom  C   45
          Population inversion found on atom  C   49
          Population inversion found on atom  C   50
          Population inversion found on atom  C   51
          Population inversion found on atom  C   62
          Population inversion found on atom  H   63
          Population inversion found on atom  H   64
          Population inversion found on atom  H   66
          Population inversion found on atom  H   71
          Population inversion found on atom  H   72
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Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.12851	1.99866	3.83690	0.03593	5.87149
O	2	-0.61101	1.99981	6.59309	0.01810	8.61101
C	3	0.02479	1.99898	3.95929	0.01694	5.97521
C	4	0.12115	1.99875	3.86161	0.01849	5.87885
C	5	0.00766	1.99898	3.97651	0.01685	5.99234
C	6	-0.22364	1.99909	4.21174	0.01281	6.22364
C	7	-0.19852	1.99920	4.18597	0.01335	6.19852
C	8	-0.22205	1.99910	4.21020	0.01275	6.22205
N	9	-0.33973	1.99944	5.32065	0.01964	7.33973
C	10	0.12972	1.99868	3.85010	0.02150	5.87028
N	11	-0.33974	1.99943	5.32037	0.01994	7.33974
C	12	-0.09948	1.99902	4.08373	0.01672	6.09948
C	13	-0.10033	1.99902	4.08462	0.01669	6.10033
B	14	0.06235	1.99770	2.92790	0.01206	4.93765
B	15	-0.16142	1.99698	3.15022	0.01422	5.16142
C	16	0.21605	1.99875	3.76261	0.02260	5.78395
N	17	-0.31003	1.99942	5.29160	0.01901	7.31003
C	18	-0.08187	1.99904	4.06665	0.01618	6.08187
C	19	-0.09119	1.99904	4.07606	0.01610	6.09119
N	20	-0.31522	1.99942	5.29648	0.01932	7.31522
C	21	0.11509	1.99873	3.86635	0.01983	5.88491
C	22	0.03333	1.99897	3.94819	0.01951	5.96667
C	23	-0.20835	1.99909	4.19618	0.01307	6.20835
C	24	-0.19335	1.99920	4.18089	0.01326	6.19335
C	25	-0.22024	1.99909	4.20856	0.01259	6.22024
C	26	0.00362	1.99898	3.98038	0.01703	5.99638
C	27	-0.25193	1.99936	4.23978	0.01279	6.25193
C	28	-0.61366	1.99941	4.60773	0.00651	6.61366
C	29	-0.24838	1.99937	4.23747	0.01154	6.24838
C	30	-0.61635	1.99942	4.61023	0.00669	6.61635
C	31	0.11991	1.99874	3.86256	0.01879	5.88009
C	32	0.01230	1.99898	3.97191	0.01681	5.98770

C	33	-0.21880	1.99910	4.20700	0.01270	6.21880
C	34	-0.19625	1.99920	4.18381	0.01324	6.19625
C	35	-0.21794	1.99909	4.20626	0.01258	6.21794
C	36	0.02057	1.99898	3.96347	0.01698	5.97943
C	37	-0.25060	1.99937	4.23978	0.01145	6.25060
C	38	-0.61786	1.99943	4.61167	0.00676	6.61786
C	39	-0.25073	1.99936	4.23974	0.01162	6.25073
C	40	-0.61509	1.99942	4.60912	0.00654	6.61509
C	41	0.11788	1.99874	3.86488	0.01850	5.88212
C	42	0.02420	1.99899	3.96030	0.01651	5.97580
C	43	-0.22241	1.99910	4.21035	0.01296	6.22241
C	44	-0.19794	1.99919	4.18527	0.01348	6.19794
C	45	-0.22485	1.99909	4.21281	0.01295	6.22485
C	46	0.00736	1.99898	3.97663	0.01702	5.99264
C	47	-0.27005	1.99935	4.25789	0.01280	6.27005
C	48	-0.61283	1.99941	4.60686	0.00656	6.61283
C	49	-0.25270	1.99937	4.24142	0.01191	6.25270
C	50	-0.61581	1.99942	4.60964	0.00675	6.61581
C	51	-0.25198	1.99937	4.24086	0.01176	6.25198
C	52	-0.61613	1.99942	4.60996	0.00675	6.61613
C	53	-0.26380	1.99935	4.25171	0.01274	6.26380
C	54	-0.61166	1.99941	4.60578	0.00647	6.61166
C	55	-0.62250	1.99942	4.61558	0.00750	6.62250
C	56	-0.62154	1.99942	4.61431	0.00781	6.62154
C	57	-0.62160	1.99943	4.61404	0.00814	6.62160
C	58	-0.61998	1.99942	4.61313	0.00744	6.61998
C	59	-0.62050	1.99942	4.61399	0.00710	6.62050
C	60	-0.62176	1.99943	4.61390	0.00843	6.62176
C	61	-0.62070	1.99942	4.61383	0.00744	6.62070
C	62	-0.63365	1.99942	4.62633	0.00790	6.63365
H	63	0.24307	0.00000	0.75545	0.00147	0.75693
H	64	0.24134	0.00000	0.75718	0.00148	0.75866
H	65	0.21351	0.00000	0.78418	0.00232	0.78649
H	66	0.21660	0.00000	0.78213	0.00126	0.78340
H	67	0.21914	0.00000	0.77872	0.00215	0.78086
H	68	0.21790	0.00000	0.77961	0.00250	0.78210
H	69	0.21869	0.00000	0.78001	0.00130	0.78131
H	70	0.21590	0.00000	0.78187	0.00224	0.78410
H	71	0.23860	0.00000	0.75987	0.00153	0.76140
H	72	0.23821	0.00000	0.76024	0.00155	0.76179
H	73	0.21223	0.00000	0.78537	0.00241	0.78777
H	74	0.21573	0.00000	0.78298	0.00130	0.78427
H	75	0.21863	0.00000	0.77911	0.00226	0.78137
H	76	0.21854	0.00000	0.77901	0.00244	0.78146
H	77	0.21520	0.00000	0.78351	0.00128	0.78480
H	78	0.21217	0.00000	0.78550	0.00233	0.78783
H	79	0.22590	0.00000	0.77152	0.00258	0.77410
H	80	0.26210	0.00000	0.73341	0.00449	0.73790
H	81	0.22511	0.00000	0.77214	0.00275	0.77489
H	82	0.25313	0.00000	0.74296	0.00391	0.74687
H	83	0.21729	0.00000	0.78007	0.00264	0.78271
H	84	0.23067	0.00000	0.76670	0.00263	0.76933
H	85	0.21917	0.00000	0.77807	0.00276	0.78083
H	86	0.22383	0.00000	0.77367	0.00250	0.77617
H	87	0.21320	0.00000	0.78542	0.00138	0.78680
H	88	0.19770	0.00000	0.80078	0.00152	0.80230
H	89	0.26129	0.00000	0.73700	0.00172	0.73871
H	90	0.21502	0.00000	0.78364	0.00134	0.78498
H	91	0.20842	0.00000	0.79026	0.00132	0.79158
H	92	0.21046	0.00000	0.78793	0.00161	0.78954
H	93	0.21461	0.00000	0.78404	0.00135	0.78539
H	94	0.21027	0.00000	0.78819	0.00153	0.78973
H	95	0.21410	0.00000	0.78467	0.00123	0.78590
H	96	0.21243	0.00000	0.78602	0.00155	0.78757
H	97	0.23875	0.00000	0.75954	0.00171	0.76125
H	98	0.20721	0.00000	0.79127	0.00152	0.79279
H	99	0.21735	0.00000	0.78131	0.00134	0.78265
H	100	0.20872	0.00000	0.78971	0.00157	0.79128
H	101	0.21299	0.00000	0.78575	0.00126	0.78701
H	102	0.21652	0.00000	0.78209	0.00138	0.78348
H	103	0.24558	0.00000	0.75294	0.00148	0.75442

H	104	0.20486	0.00000	0.79353	0.00160	0.79514
H	105	0.21737	0.00000	0.78132	0.00131	0.78263
H	106	0.21608	0.00000	0.78269	0.00123	0.78392
H	107	0.20821	0.00000	0.79026	0.00153	0.79179
H	108	0.21386	0.00000	0.78460	0.00154	0.78614
H	109	0.20828	0.00000	0.79003	0.00170	0.79172
H	110	0.24298	0.00000	0.75556	0.00146	0.75702
H	111	0.21175	0.00000	0.78672	0.00153	0.78825
H	112	0.20542	0.00000	0.79290	0.00168	0.79458
H	113	0.23486	0.00000	0.76404	0.00111	0.76514
H	114	0.21445	0.00000	0.78418	0.00136	0.78555
H	115	0.21635	0.00000	0.78240	0.00124	0.78365
H	116	0.20845	0.00000	0.79000	0.00156	0.79155
H	117	0.21805	0.00000	0.78063	0.00132	0.78195
H	118	0.20603	0.00000	0.79236	0.00161	0.79397
H	119	0.21019	0.00000	0.78849	0.00133	0.78981
H	120	0.22945	0.00000	0.76926	0.00129	0.77055
H	121	0.23485	0.00000	0.76360	0.00156	0.76515
H	122	0.19322	0.00000	0.80520	0.00158	0.80678
H	123	0.23063	0.00000	0.76792	0.00144	0.76937
H	124	0.19600	0.00000	0.80245	0.00155	0.80400
H	125	0.22607	0.00000	0.77264	0.00129	0.77393
H	126	0.21880	0.00000	0.77990	0.00131	0.78120
H	127	0.21257	0.00000	0.78610	0.00133	0.78743
H	128	0.20518	0.00000	0.79321	0.00161	0.79482
H	129	0.21449	0.00000	0.78416	0.00135	0.78551
H	130	0.20848	0.00000	0.78995	0.00156	0.79152
H	131	0.21577	0.00000	0.78295	0.00128	0.78423
H	132	0.21281	0.00000	0.78564	0.00154	0.78719
H	133	0.23566	0.00000	0.76264	0.00170	0.76434
H	134	0.20324	0.00000	0.79518	0.00158	0.79676
* Total *		0.00000	123.94637	323.08119	0.97245	448.00000

Natural Population

Core	123.94637	(99.9567% of 124)
Valence	323.08119	(99.7164% of 324)
Natural Minimal Basis	447.02755	(99.7829% of 448)
Natural Rydberg Basis	0.97245	(0.2171% of 448)

Atom	No	Natural Electron Configuration
C	1	[core]2S(0.91)2p(2.92)3S(0.01)3p(0.02)3d(0.01)
O	2	[core]2S(1.70)2p(4.89)3p(0.01)
C	3	[core]2S(0.93)2p(3.03)3p(0.01)
C	4	[core]2S(0.87)2p(2.99)3p(0.01)
C	5	[core]2S(0.92)2p(3.05)3p(0.01)
C	6	[core]2S(0.97)2p(3.24)
C	7	[core]2S(0.98)2p(3.21)3p(0.01)
C	8	[core]2S(0.97)2p(3.24)3p(0.01)
N	9	[core]2S(1.19)2p(4.13)3p(0.01)
C	10	[core]2S(0.95)2p(2.90)3p(0.01)4p(0.01)
N	11	[core]2S(1.19)2p(4.13)3p(0.01)
C	12	[core]2S(0.95)2p(3.13)3p(0.01)
C	13	[core]2S(0.95)2p(3.13)3p(0.01)
B	14	[core]2S(0.66)2p(2.26)
B	15	[core]2S(0.62)2p(2.53)
C	16	[core]2S(0.95)2p(2.81)3p(0.01)4p(0.01)
N	17	[core]2S(1.20)2p(4.10)3p(0.01)
C	18	[core]2S(0.95)2p(3.11)3p(0.01)
C	19	[core]2S(0.96)2p(3.12)3p(0.01)
N	20	[core]2S(1.19)2p(4.10)3p(0.01)
C	21	[core]2S(0.87)2p(3.00)3p(0.01)
C	22	[core]2S(0.92)2p(3.03)3p(0.01)
C	23	[core]2S(0.97)2p(3.22)
C	24	[core]2S(0.98)2p(3.20)3p(0.01)
C	25	[core]2S(0.97)2p(3.24)3p(0.01)
C	26	[core]2S(0.92)2p(3.06)3p(0.01)
C	27	[core]2S(1.00)2p(3.24)3p(0.01)

```
C   28      [core]2S( 1.12)2p( 3.49)
C   29      [core]2S( 1.00)2p( 3.24)3p( 0.01)
C   30      [core]2S( 1.12)2p( 3.49)
C   31      [core]2S( 0.87)2p( 3.00)3p( 0.01)
C   32      [core]2S( 0.92)2p( 3.05)3p( 0.01)
C   33      [core]2S( 0.97)2p( 3.23)3p( 0.01)
C   34      [core]2S( 0.98)2p( 3.21)3p( 0.01)
C   35      [core]2S( 0.97)2p( 3.23)3p( 0.01)
C   36      [core]2S( 0.92)2p( 3.04)3p( 0.01)
C   37      [core]2S( 1.00)2p( 3.24)3p( 0.01)
C   38      [core]2S( 1.11)2p( 3.50)
C   39      [core]2S( 1.00)2p( 3.24)3p( 0.01)
C   40      [core]2S( 1.12)2p( 3.49)
C   41      [core]2S( 0.87)2p( 3.00)3p( 0.01)
C   42      [core]2S( 0.93)2p( 3.03)3p( 0.01)
C   43      [core]2S( 0.97)2p( 3.24)3p( 0.01)
C   44      [core]2S( 0.98)2p( 3.21)3p( 0.01)
C   45      [core]2S( 0.97)2p( 3.24)3p( 0.01)
C   46      [core]2S( 0.92)2p( 3.05)3p( 0.01)
C   47      [core]2S( 1.00)2p( 3.26)3p( 0.01)
C   48      [core]2S( 1.12)2p( 3.49)
C   49      [core]2S( 1.00)2p( 3.25)3p( 0.01)
C   50      [core]2S( 1.12)2p( 3.49)
C   51      [core]2S( 1.00)2p( 3.24)3p( 0.01)
C   52      [core]2S( 1.12)2p( 3.49)
C   53      [core]2S( 1.00)2p( 3.25)3p( 0.01)
C   54      [core]2S( 1.12)2p( 3.49)
C   55      [core]2S( 1.12)2p( 3.50)
C   56      [core]2S( 1.11)2p( 3.50)
C   57      [core]2S( 1.11)2p( 3.50)
C   58      [core]2S( 1.11)2p( 3.50)
C   59      [core]2S( 1.11)2p( 3.50)
C   60      [core]2S( 1.11)2p( 3.50)
C   61      [core]2S( 1.12)2p( 3.50)
C   62      [core]2S( 1.11)2p( 3.51)
H   63            1S( 0.76)
H   64            1S( 0.76)
H   65            1S( 0.78)
H   66            1S( 0.78)
H   67            1S( 0.78)
H   68            1S( 0.78)
H   69            1S( 0.78)
H   70            1S( 0.78)
H   71            1S( 0.76)
H   72            1S( 0.76)
H   73            1S( 0.79)
H   74            1S( 0.78)
H   75            1S( 0.78)
H   76            1S( 0.78)
H   77            1S( 0.78)
H   78            1S( 0.79)
H   79            1S( 0.77)
H   80            1S( 0.73)
H   81            1S( 0.77)
H   82            1S( 0.74)
H   83            1S( 0.78)
H   84            1S( 0.77)
H   85            1S( 0.78)
H   86            1S( 0.77)
H   87            1S( 0.79)
H   88            1S( 0.80)
H   89            1S( 0.74)
H   90            1S( 0.78)
H   91            1S( 0.79)
H   92            1S( 0.79)
H   93            1S( 0.78)
H   94            1S( 0.79)
H   95            1S( 0.78)
H   96            1S( 0.79)
H   97            1S( 0.76)
H   98            1S( 0.79)
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     H   99            1S( 0.78)
     H  100            1S( 0.79)
     H  101            1S( 0.79)
     H  102            1S( 0.78)
     H  103            1S( 0.75)
     H  104            1S( 0.79)
     H  105            1S( 0.78)
     H  106            1S( 0.78)
     H  107            1S( 0.79)
     H  108            1S( 0.78)
     H  109            1S( 0.79)
     H  110            1S( 0.76)
     H  111            1S( 0.79)
     H  112            1S( 0.79)
     H  113            1S( 0.76)
     H  114            1S( 0.78)
     H  115            1S( 0.78)
     H  116            1S( 0.79)
     H  117            1S( 0.78)
     H  118            1S( 0.79)
     H  119            1S( 0.79)
     H  120            1S( 0.77)
     H  121            1S( 0.76)
     H  122            1S( 0.81)
     H  123            1S( 0.77)
     H  124            1S( 0.80)
     H  125            1S( 0.77)
     H  126            1S( 0.78)
     H  127            1S( 0.79)
     H  128            1S( 0.79)
     H  129            1S( 0.78)
     H  130            1S( 0.79)
     H  131            1S( 0.78)
     H  132            1S( 0.79)
     H  133            1S( 0.76)
     H  134            1S( 0.80)
```

NATURAL BOND ORBITAL ANALYSIS:

Cycle	Occ. Thresh.	Occupancies Lewis	Occupancies Non-Lewis	Lewis Structure CR	BD	3C	LP	Low occ (L)	High occ (NL)	Dev
1(1)	1.90	426.68707	21.31293	62	140	0	22	21	21	1.25
2(2)	1.90	426.68707	21.31293	62	140	0	22	21	21	1.25
3(1)	1.80	429.54420	18.45580	62	145	0	17	16	19	0.89
4(2)	1.80	429.54420	18.45580	62	145	0	17	16	19	0.89
5(1)	1.70	429.45121	18.54879	62	144	0	18	16	19	0.89
6(2)	1.70	429.45121	18.54879	62	144	0	18	16	19	0.89
7(1)	1.60	436.90072	11.09928	62	158	0	4	2	20	0.44
8(2)	1.60	436.49078	11.50922	62	157	0	5	3	20	0.44
9(3)	1.60	436.90072	11.09928	62	158	0	4	2	20	0.44
10(1)	1.50	436.58556	11.41444	62	154	0	8	1	19	0.55
11(2)	1.50	436.58556	11.41444	62	154	0	8	1	19	0.55
12(1)	1.60	436.90072	11.09928	62	158	0	4	2	20	0.44

Structure accepted: RESONANCE keyword permits strongly delocalized structure

```
WARNING:  1 low occupancy (<1.9990e) core orbital  found on  C    1
          1 low occupancy (<1.9990e) core orbital  found on  C    3
          1 low occupancy (<1.9990e) core orbital  found on  C    4
          1 low occupancy (<1.9990e) core orbital  found on  C    5
          1 low occupancy (<1.9990e) core orbital  found on  C   10
          1 low occupancy (<1.9990e) core orbital  found on  B   14
          1 low occupancy (<1.9990e) core orbital  found on  B   15
          1 low occupancy (<1.9990e) core orbital  found on  C   16
          1 low occupancy (<1.9990e) core orbital  found on  C   21
          1 low occupancy (<1.9990e) core orbital  found on  C   22
          1 low occupancy (<1.9990e) core orbital  found on  C   26
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          1 low occupancy (<1.9990e) core orbital  found on  C   31
          1 low occupancy (<1.9990e) core orbital  found on  C   32
          1 low occupancy (<1.9990e) core orbital  found on  C   36
          1 low occupancy (<1.9990e) core orbital  found on  C   41
          1 low occupancy (<1.9990e) core orbital  found on  C   42
          1 low occupancy (<1.9990e) core orbital  found on  C   46

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  Core                   123.94632 ( 99.957% of 124)
  Valence Lewis          312.95441 ( 96.591% of 324)
 ==================      ============================
  Total Lewis            436.90072 ( 97.522% of 448)
 -------------------------------------------------------
  Valence non-Lewis       10.37751 (  2.316% of 448)
  Rydberg non-Lewis        0.72177 (  0.161% of 448)
 ==================      ============================
  Total non-Lewis         11.09928 (  2.478% of 448)
-------------------------------------------------------


      (Occupancy)   Bond orbital/ Coefficients/ Hybrids
-------------------------------------------------------------------------------
    1. (1.99525) BD ( 1) C   1 - O   2
               ( 35.42%)   0.5952* C   1 s( 34.37%)p 1.91( 65.56%)d 0.00(  0.06%)
                                        -0.0003  0.5810  0.0787  0.0026  0.0008
                                        -0.1509  0.0180 -0.0037  0.2199 -0.0122
                                         0.0042 -0.7618  0.0561 -0.0225 -0.0018
                                         0.0052 -0.0118 -0.0016  0.0209
               ( 64.58%)   0.8036* O   2 s( 39.92%)p 1.50( 59.94%)d 0.00(  0.14%)
                                         0.0000  0.6315 -0.0188  0.0010  0.0004
                                         0.1663 -0.0065  0.0004 -0.1629  0.0093
                                        -0.0006  0.7377 -0.0308  0.0019 -0.0037
                                         0.0129 -0.0137 -0.0010  0.0316
    2. (1.98559) BD ( 2) C   1 - O   2
               ( 26.78%)   0.5175* C   1 s(  0.01%)p99.99( 99.72%)d18.73(  0.27%)
                                         0.0002 -0.0112 -0.0035 -0.0020 -0.0003
                                        -0.2669  0.0057  0.0009  0.9119 -0.0046
                                         0.0006  0.3072 -0.0019  0.0018 -0.0103
                                         0.0104 -0.0412 -0.0105 -0.0253
               ( 73.22%)   0.8557* O   2 s(  0.02%)p99.99( 99.88%)d 5.56(  0.10%)
                                         0.0000 -0.0134 -0.0014 -0.0001  0.0000
                                        -0.2373  0.0040  0.0009  0.9322 -0.0117
                                        -0.0030  0.2709 -0.0019 -0.0007  0.0081
                                        -0.0058  0.0259  0.0058  0.0143
    3. (1.68991) BD ( 1) C   1 - B  14
               ( 60.05%)   0.7749* C   1 s( 25.83%)p 2.87( 74.14%)d 0.00(  0.03%)
                                        -0.0001  0.5076 -0.0246 -0.0070 -0.0004
                                         0.8031  0.0080 -0.0050  0.1500 -0.0005
                                         0.0048  0.2708  0.0196 -0.0097  0.0031
                                         0.0135 -0.0001  0.0090  0.0021
               ( 39.95%)   0.6321* B  14 s( 18.02%)p 4.55( 81.92%)d 0.00(  0.06%)
                                        -0.0048  0.4244  0.0071 -0.0015 -0.0003
                                        -0.4109  0.0053 -0.0033  0.0158  0.0057
                                         0.0025 -0.8062 -0.0060 -0.0081  0.0063
                                         0.0176 -0.0066  0.0089  0.0131
    4. (1.86978) BD ( 1) C   1 - B  15
               ( 60.99%)   0.7810* C   1 s( 40.15%)p 1.49( 59.83%)d 0.00(  0.02%)
                                         0.0001 -0.6328  0.0332 -0.0034  0.0001
                                         0.5101  0.0005  0.0070  0.3077  0.0062
                                         0.0019 -0.4931 -0.0133  0.0081 -0.0030
                                         0.0054  0.0082  0.0022 -0.0088
               ( 39.01%)   0.6246* B  15 s( 26.26%)p 2.81( 73.68%)d 0.00(  0.06%)
                                         0.0013 -0.5124  0.0006 -0.0061 -0.0024
                                         0.1733  0.0148  0.0020 -0.2436  0.0080
                                        -0.0044  0.8041 -0.0048  0.0218 -0.0056
                                        -0.0010  0.0151  0.0019 -0.0182
    5. (1.96959) BD ( 1) C   3 - C   4
               ( 49.25%)   0.7018* C   3 s( 33.55%)p 1.98( 66.40%)d 0.00(  0.05%)
                                         0.0000  0.5792  0.0032 -0.0011  0.0000
                                         0.6350  0.0004  0.0019 -0.3736  0.0069
                                        -0.0003  0.3477  0.0118 -0.0009 -0.0140
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                                      0.0145 -0.0072  0.0091 -0.0030
           ( 50.75%)   0.7124* C   4 s( 36.74%)p 1.72( 63.22%)d 0.00(  0.05%)
                                     -0.0002  0.6061 -0.0011 -0.0031  0.0001
                                     -0.6195 -0.0040  0.0023  0.3295  0.0077
                                      0.0040 -0.3739  0.0032  0.0010 -0.0129
                                      0.0138 -0.0072  0.0075 -0.0019
 6. (1.97359) BD ( 1) C   3 - C   8
           ( 50.42%)   0.7101* C   3 s( 34.07%)p 1.93( 65.88%)d 0.00(  0.05%)
                                     -0.0001  0.5836  0.0091  0.0048  0.0002
                                     -0.4788  0.0077 -0.0076  0.4929 -0.0029
                                      0.0080  0.4318  0.0076 -0.0010 -0.0138
                                     -0.0104  0.0129 -0.0009  0.0007
           ( 49.58%)   0.7041* C   8 s( 35.90%)p 1.78( 64.04%)d 0.00(  0.06%)
                                      0.0001  0.5992 -0.0007 -0.0043 -0.0002
                                      0.4507 -0.0025 -0.0059 -0.4802 -0.0069
                                      0.0071 -0.4539 -0.0196  0.0025 -0.0166
                                     -0.0120  0.0142  0.0003 -0.0001
 7. (1.63548) BD ( 2) C   3 - C   8
           ( 47.79%)   0.6913* C   3 s(  0.01%)p 1.00( 99.96%)d 0.00(  0.04%)
                                     -0.0002 -0.0061 -0.0052  0.0017  0.0003
                                      0.5871 -0.0051 -0.0041  0.7766 -0.0049
                                      0.0038 -0.2274  0.0013  0.0034  0.0020
                                      0.0102  0.0115 -0.0080 -0.0077
           ( 52.21%)   0.7226* C   8 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                      0.0000 -0.0005  0.0012 -0.0001  0.0005
                                      0.5811 -0.0025  0.0077  0.7759 -0.0046
                                      0.0117 -0.2444  0.0029 -0.0050  0.0039
                                     -0.0044  0.0011  0.0165  0.0008
 8. (1.96975) BD ( 1) C   3 - C  53
           ( 50.58%)   0.7112* C   3 s( 32.34%)p 2.09( 67.63%)d 0.00(  0.03%)
                                     -0.0001  0.5687 -0.0066 -0.0047 -0.0002
                                     -0.1492 -0.0019 -0.0020 -0.1170  0.0003
                                      0.0019 -0.8000 -0.0171  0.0075 -0.0010
                                      0.0041  0.0037  0.0004  0.0167
           ( 49.42%)   0.7030* C  53 s( 26.35%)p 2.79( 73.59%)d 0.00(  0.06%)
                                      0.0002  0.5134 -0.0001  0.0003  0.0007
                                      0.1312 -0.0019 -0.0018  0.1039 -0.0049
                                      0.0005  0.8413 -0.0005  0.0012  0.0017
                                      0.0071  0.0055  0.0001  0.0222
 9. (1.96881) BD ( 1) C   4 - C   5
           ( 50.40%)   0.7100* C   4 s( 36.67%)p 1.73( 63.29%)d 0.00(  0.05%)
                                     -0.0002  0.6055 -0.0021 -0.0024  0.0002
                                      0.1961 -0.0018  0.0000  0.1188  0.0073
                                      0.0029  0.7617  0.0054  0.0009  0.0001
                                      0.0098  0.0064  0.0016  0.0184
           ( 49.60%)   0.7043* C   5 s( 34.19%)p 1.92( 65.76%)d 0.00(  0.05%)
                                      0.0000  0.5847  0.0024 -0.0005  0.0000
                                     -0.1664 -0.0103  0.0024 -0.1615  0.0086
                                     -0.0002 -0.7770 -0.0013  0.0000 -0.0001
                                      0.0093  0.0063  0.0014  0.0199
10. (1.66564) BD ( 2) C   4 - C   5
           ( 53.47%)   0.7313* C   4 s(  0.01%)p 1.00( 99.97%)d 0.00(  0.02%)
                                     -0.0002 -0.0074 -0.0051  0.0012  0.0002
                                      0.5662 -0.0040 -0.0069  0.7814 -0.0019
                                     -0.0052 -0.2617  0.0052  0.0035  0.0036
                                      0.0068  0.0089 -0.0036 -0.0072
           ( 46.53%)   0.6821* C   5 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                      0.0000 -0.0033 -0.0047  0.0017  0.0001
                                      0.5493 -0.0052 -0.0024  0.7857 -0.0081
                                     -0.0027 -0.2835  0.0007 -0.0017 -0.0075
                                     -0.0073 -0.0147 -0.0077  0.0082
11. (1.98185) BD ( 1) C   4 - N   9
           ( 37.66%)   0.6136* C   4 s( 26.55%)p 2.76( 73.39%)d 0.00(  0.06%)
                                     -0.0002  0.5151  0.0074  0.0066 -0.0005
                                      0.5066  0.0050  0.0081 -0.5159 -0.0055
                                     -0.0090 -0.4593  0.0016 -0.0076 -0.0161
                                     -0.0134  0.0140  0.0008 -0.0009
           ( 62.34%)   0.7896* N   9 s( 34.35%)p 1.91( 65.61%)d 0.00(  0.04%)
                                     -0.0001  0.5861  0.0014 -0.0018 -0.0002
                                     -0.5033 -0.0022  0.0070  0.4858  0.0043
                                     -0.0067  0.4082 -0.0003 -0.0048 -0.0105
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                                    -0.0123  0.0112 -0.0002 -0.0016
12. (1.97300) BD ( 1) C   5 - C   6
            ( 50.49%)   0.7106* C   5 s( 33.92%)p 1.95( 66.03%)d 0.00(  0.05%)
                                    -0.0001  0.5823  0.0106  0.0031  0.0001
                                    -0.4752 -0.0025 -0.0010  0.4927 -0.0003
                                     0.0048  0.4376 -0.0094  0.0090 -0.0150
                                    -0.0100  0.0120  0.0004 -0.0013
            ( 49.51%)   0.7036* C   6 s( 35.81%)p 1.79( 64.13%)d 0.00(  0.06%)
                                     0.0001  0.5984 -0.0016 -0.0044 -0.0001
                                     0.4925  0.0164 -0.0051 -0.4866 -0.0112
                                     0.0066 -0.4018  0.0051  0.0076 -0.0168
                                    -0.0117  0.0137  0.0007 -0.0004
13. (1.96978) BD ( 1) C   5 - C  51
            ( 50.02%)   0.7072* C   5 s( 31.86%)p 2.14( 68.11%)d 0.00(  0.03%)
                                    -0.0001  0.5644 -0.0069 -0.0033  0.0000
                                     0.6662  0.0130 -0.0046 -0.3364 -0.0053
                                     0.0026  0.3517  0.0096 -0.0018 -0.0105
                                     0.0103 -0.0041  0.0084 -0.0036
            ( 49.98%)   0.7070* C  51 s( 26.67%)p 2.75( 73.28%)d 0.00(  0.06%)
                                     0.0001  0.5164  0.0015 -0.0019 -0.0002
                                    -0.7022  0.0010  0.0024  0.3264 -0.0035
                                     0.0000 -0.3649 -0.0009  0.0026 -0.0128
                                     0.0144 -0.0069  0.0104 -0.0054
14. (1.98099) BD ( 1) C   6 - C   7
            ( 50.22%)   0.7086* C   6 s( 36.09%)p 1.77( 63.85%)d 0.00(  0.05%)
                                     0.0000  0.6006  0.0147  0.0044  0.0001
                                    -0.6446 -0.0175 -0.0032  0.3477  0.0183
                                     0.0066 -0.3178  0.0155  0.0120 -0.0115
                                     0.0161 -0.0067  0.0089 -0.0006
            ( 49.78%)   0.7056* C   7 s( 35.95%)p 1.78( 63.98%)d 0.00(  0.07%)
                                     0.0000  0.5996  0.0077 -0.0016 -0.0001
                                     0.6232  0.0103 -0.0093 -0.3357  0.0025
                                     0.0091  0.3708  0.0309  0.0057 -0.0182
                                     0.0120 -0.0058  0.0096 -0.0073
15. (1.67366) BD ( 2) C   6 - C   7
            ( 51.04%)   0.7144* C   6 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                                     0.0000  0.0015 -0.0002  0.0006  0.0001
                                     0.5570 -0.0058  0.0136  0.7859 -0.0076
                                     0.0176 -0.2669  0.0028 -0.0054 -0.0053
                                    -0.0049 -0.0103 -0.0058  0.0060
            ( 48.96%)   0.6997* C   7 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                     0.0000  0.0039  0.0000  0.0013  0.0001
                                     0.5698 -0.0063  0.0060  0.7800 -0.0074
                                     0.0096 -0.2578  0.0028 -0.0028  0.0044
                                    -0.0034  0.0027  0.0148  0.0002
16. (1.97545) BD ( 1) C   6 - H  78
            ( 60.76%)   0.7795* C   6 s( 28.07%)p 2.56( 71.90%)d 0.00(  0.04%)
                                    -0.0004  0.5297 -0.0109 -0.0003  0.0001
                                     0.1735 -0.0082 -0.0044  0.1530  0.0002
                                    -0.0007  0.8155 -0.0142 -0.0126  0.0010
                                     0.0071  0.0057  0.0003  0.0168
            ( 39.24%)   0.6264* H  78 s( 99.95%)p 0.00(  0.05%)
                                     0.9997  0.0022  0.0013 -0.0050 -0.0040
                                    -0.0222
17. (1.98085) BD ( 1) C   7 - C   8
            ( 49.96%)   0.7069* C   7 s( 36.04%)p 1.77( 63.89%)d 0.00(  0.06%)
                                     0.0000  0.6003  0.0063 -0.0024 -0.0002
                                    -0.1853 -0.0243 -0.0055 -0.1213  0.0118
                                     0.0094 -0.7672 -0.0174  0.0095 -0.0005
                                     0.0050  0.0105 -0.0005  0.0226
            ( 50.04%)   0.7074* C   8 s( 35.83%)p 1.79( 64.12%)d 0.00(  0.05%)
                                     0.0000  0.5984  0.0139  0.0046  0.0002
                                     0.1372 -0.0176 -0.0093  0.1417  0.0186
                                     0.0098  0.7754  0.0163  0.0012 -0.0001
                                     0.0115  0.0031  0.0019  0.0191
18. (1.97757) BD ( 1) C   7 - H  77
            ( 60.84%)   0.7800* C   7 s( 27.95%)p 2.58( 72.01%)d 0.00(  0.03%)
                                     0.0004 -0.5286  0.0118 -0.0036 -0.0003
                                     0.5010 -0.0133  0.0018 -0.5131  0.0144
                                    -0.0026 -0.4530  0.0128 -0.0024  0.0076
                                     0.0127 -0.0092  0.0020  0.0041
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            ( 39.16%)   0.6258* H  77 s( 99.95%)p 0.00(  0.05%)
                                      -0.9997 -0.0015 -0.0005 -0.0136  0.0141
                                       0.0123
19. (1.97490) BD ( 1) C   8 - H  76
            ( 61.08%)   0.7816* C   8 s( 28.24%)p 2.54( 71.73%)d 0.00(  0.04%)
                                       0.0004 -0.5313  0.0108  0.0006 -0.0001
                                       0.6628 -0.0102 -0.0096 -0.3826  0.0062
                                       0.0030  0.3622 -0.0106 -0.0065  0.0115
                                      -0.0112  0.0063 -0.0070  0.0039
            ( 38.92%)   0.6238* H  76 s( 99.95%)p 0.00(  0.05%)
                                      -0.9997  0.0020 -0.0015 -0.0184  0.0096
                                      -0.0106
20. (1.97311) BD ( 1) N   9 - C  10
            ( 62.47%)   0.7904* N   9 s( 33.77%)p 1.96( 66.17%)d 0.00(  0.05%)
                                       0.0001 -0.5812  0.0006 -0.0005 -0.0001
                                       0.1567 -0.0128  0.0030  0.7937 -0.0065
                                      -0.0042  0.0829  0.0075 -0.0023 -0.0033
                                       0.0015 -0.0045  0.0191  0.0116
            ( 37.53%)   0.6126* C  10 s( 26.30%)p 2.80( 73.64%)d 0.00(  0.06%)
                                       0.0004 -0.5123 -0.0205 -0.0092  0.0005
                                      -0.0496  0.0115  0.0041 -0.8485 -0.0207
                                      -0.0158 -0.1141 -0.0057 -0.0065 -0.0078
                                       0.0005 -0.0007  0.0195  0.0135
21. (1.85857) BD ( 2) N   9 - C  10
            ( 76.19%)   0.8729* N   9 s(  0.08%)p99.99( 99.90%)d 0.16(  0.01%)
                                      -0.0001 -0.0286  0.0055 -0.0002  0.0000
                                       0.4677  0.0066  0.0033 -0.2030 -0.0001
                                      -0.0017  0.8596  0.0076  0.0085 -0.0057
                                       0.0023 -0.0086  0.0003 -0.0047
            ( 23.81%)   0.4879* C  10 s(  0.09%)p99.99( 99.74%)d 1.76(  0.17%)
                                       0.0003  0.0299  0.0060 -0.0037  0.0003
                                       0.4290 -0.0003  0.0060 -0.1623 -0.0095
                                       0.0087  0.8865  0.0299 -0.0064  0.0161
                                       0.0117  0.0336  0.0113  0.0020
22. (1.97621) BD ( 1) N   9 - C  13
            ( 61.98%)   0.7873* N   9 s( 31.75%)p 2.15( 68.20%)d 0.00(  0.05%)
                                      -0.0001  0.5634 -0.0047  0.0013  0.0001
                                       0.7088 -0.0056 -0.0011  0.3030 -0.0236
                                       0.0050 -0.2953  0.0059 -0.0005  0.0098
                                      -0.0129 -0.0026  0.0134 -0.0081
            ( 38.02%)   0.6166* C  13 s( 28.26%)p 2.54( 71.68%)d 0.00(  0.05%)
                                      -0.0001  0.5316  0.0032  0.0003 -0.0016
                                      -0.7547 -0.0287 -0.0054 -0.1846  0.0096
                                       0.0080  0.3346  0.0139 -0.0005  0.0120
                                      -0.0141 -0.0041  0.0101 -0.0092
23. (1.97446) BD ( 1) C  10 - N  11
            ( 37.53%)   0.6126* C  10 s( 26.68%)p 2.75( 73.25%)d 0.00(  0.07%)
                                       0.0003 -0.5161 -0.0213 -0.0043 -0.0005
                                      -0.6918 -0.0103 -0.0069  0.2967  0.0190
                                       0.0109  0.4064  0.0119  0.0035  0.0066
                                       0.0197 -0.0043 -0.0148  0.0043
            ( 62.47%)   0.7904* N  11 s( 34.03%)p 1.94( 65.91%)d 0.00(  0.05%)
                                       0.0001 -0.5834  0.0016  0.0010 -0.0001
                                       0.7080 -0.0084 -0.0014 -0.1705 -0.0128
                                       0.0062 -0.3585  0.0042  0.0015  0.0095
                                       0.0166 -0.0055 -0.0109  0.0048
24. (1.96616) BD ( 1) C  10 - B  14
            ( 66.78%)   0.8172* C  10 s( 46.95%)p 1.13( 53.05%)d 0.00(  0.01%)
                                       0.0001 -0.6850  0.0155  0.0068  0.0001
                                       0.5768 -0.0305 -0.0040  0.4040 -0.0161
                                      -0.0044 -0.1823  0.0052  0.0044 -0.0050
                                       0.0025 -0.0008 -0.0025  0.0069
            ( 33.22%)   0.5763* B  14 s( 40.37%)p 1.48( 59.58%)d 0.00(  0.05%)
                                       0.0004 -0.6352  0.0007 -0.0122 -0.0023
                                      -0.6817 -0.0097 -0.0209 -0.3609 -0.0041
                                      -0.0118  0.0061 -0.0050 -0.0015 -0.0169
                                       0.0041  0.0030 -0.0093  0.0109
25. (1.97540) BD ( 1) N  11 - C  12
            ( 61.97%)   0.7872* N  11 s( 31.51%)p 2.17( 68.44%)d 0.00(  0.05%)
                                      -0.0001  0.5613 -0.0035 -0.0002  0.0001
                                       0.5370 -0.0192  0.0027  0.6123 -0.0020
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                                    -0.0030 -0.1432  0.0151 -0.0031  0.0183
                                    -0.0038 -0.0031 -0.0049 -0.0122
            ( 38.03%)   0.6167* C  12 s( 28.22%)p 2.54( 71.71%)d 0.00(  0.06%)
                                    -0.0001  0.5312  0.0034  0.0015 -0.0012
                                    -0.4570 -0.0049  0.0039 -0.7044 -0.0333
                                    -0.0062  0.1045 -0.0039 -0.0063  0.0193
                                    -0.0078 -0.0050 -0.0033 -0.0130
26. (1.98143) BD ( 1) N  11 - C  41
            ( 62.37%)   0.7897* N  11 s( 34.36%)p 1.91( 65.60%)d 0.00(  0.04%)
                                    -0.0001  0.5862  0.0010  0.0012 -0.0002
                                     0.2057  0.0034 -0.0033 -0.7610 -0.0028
                                     0.0091 -0.1858 -0.0035  0.0033 -0.0086
                                    -0.0031  0.0054 -0.0132 -0.0101
            ( 37.63%)   0.6135* C  41 s( 26.52%)p 2.77( 73.36%)d 0.00(  0.12%)
                                    -0.0002  0.5149  0.0047  0.0051 -0.0006
                                    -0.2723 -0.0053  0.0002  0.7932 -0.0014
                                     0.0077  0.1726 -0.0195  0.0063 -0.0216
                                     0.0013 -0.0086 -0.0195 -0.0170
27. (1.60454) BD ( 2) N  11 - C  41
            ( 98.46%)   0.9923* N  11 s(  0.05%)p99.99( 99.95%)d 0.07(  0.00%)
                                    -0.0002 -0.0219  0.0041  0.0000  0.0000
                                     0.4088  0.0051  0.0039 -0.1270  0.0003
                                    -0.0017  0.9034  0.0040  0.0089  0.0025
                                     0.0014  0.0047  0.0000  0.0026
            (  1.54%)   0.1241* C  41 s(  1.14%)p58.44( 66.45%)d28.50( 32.41%)
                                     0.0006  0.0261  0.0961  0.0380  0.0044
                                     0.2042  0.1381 -0.0950 -0.0584 -0.0396
                                     0.0642  0.6365  0.4107 -0.1088  0.2537
                                    -0.0832  0.4746  0.0335  0.1627
28. (1.97682) BD ( 1) C  12 - C  13
            ( 49.99%)   0.7070* C  12 s( 37.54%)p 1.66( 62.40%)d 0.00(  0.05%)
                                     0.0000  0.6126  0.0104  0.0031  0.0006
                                    -0.2903  0.0129  0.0145  0.6870  0.0316
                                     0.0095  0.2575 -0.0015 -0.0065 -0.0138
                                    -0.0098  0.0116 -0.0063 -0.0088
            ( 50.01%)   0.7072* C  13 s( 37.53%)p 1.66( 62.42%)d 0.00(  0.05%)
                                     0.0000  0.6125  0.0100  0.0033  0.0007
                                     0.4344  0.0312  0.0123 -0.5810  0.0004
                                     0.0120 -0.3106 -0.0146 -0.0068 -0.0117
                                    -0.0077  0.0113 -0.0105 -0.0100
29. (1.91018) BD ( 2) C  12 - C  13
            ( 50.00%)   0.7071* C  12 s(  0.00%)p 1.00( 99.94%)d 0.00(  0.06%)
                                     0.0000 -0.0008 -0.0050  0.0014  0.0001
                                     0.4327 -0.0088 -0.0005 -0.1495  0.0032
                                     0.0009  0.8884 -0.0214  0.0006  0.0094
                                    -0.0085  0.0127 -0.0041  0.0156
            ( 50.00%)   0.7071* C  13 s(  0.00%)p 1.00( 99.94%)d 0.00(  0.06%)
                                     0.0000  0.0009 -0.0060  0.0030  0.0001
                                     0.4317 -0.0092  0.0002 -0.1515  0.0050
                                    -0.0009  0.8886 -0.0207 -0.0004 -0.0107
                                     0.0030 -0.0186  0.0000 -0.0108
30. (1.97879) BD ( 1) C  12 - H  71
            ( 61.95%)   0.7871* C  12 s( 34.17%)p 1.93( 65.81%)d 0.00(  0.02%)
                                    -0.0003  0.5845 -0.0079 -0.0037  0.0002
                                     0.7203 -0.0114  0.0016 -0.0807  0.0051
                                     0.0116 -0.3639  0.0070  0.0004 -0.0028
                                    -0.0105  0.0017  0.0096 -0.0034
            ( 38.05%)   0.6168* H  71 s( 99.93%)p 0.00(  0.07%)
                                     0.9997  0.0018  0.0002 -0.0228  0.0029
                                     0.0117
31. (1.97878) BD ( 1) C  13 - H  72
            ( 61.94%)   0.7870* C  13 s( 34.15%)p 1.93( 65.83%)d 0.00(  0.02%)
                                    -0.0003  0.5843 -0.0076 -0.0032  0.0005
                                     0.2301 -0.0005  0.0092  0.7776 -0.0141
                                    -0.0024  0.0202 -0.0012 -0.0069  0.0068
                                    -0.0005  0.0012 -0.0107 -0.0079
            ( 38.06%)   0.6169* H  72 s( 99.93%)p 0.00(  0.07%)
                                     0.9997  0.0018  0.0003 -0.0071 -0.0249
                                    -0.0005
32. (1.82710) BD ( 1) B  14 - B  15
            ( 50.00%)   0.7071* B  14 s( 41.46%)p 1.41( 58.51%)d 0.00(  0.02%)
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                                     0.0003  0.6439  0.0009 -0.0079 -0.0014
                                    -0.3842 -0.0057  0.0086 -0.3996  0.0034
                                     0.0018  0.5269 -0.0074  0.0050  0.0076
                                     0.0007  0.0047  0.0094 -0.0089
            ( 50.00%)   0.7071* B  15 s( 35.85%)p 1.79( 64.13%)d 0.00(  0.02%)
                                     0.0005  0.5986  0.0042 -0.0098 -0.0020
                                     0.7256 -0.0099 -0.0112  0.1869 -0.0087
                                    -0.0056  0.2817  0.0076  0.0063  0.0093
                                    -0.0066 -0.0034  0.0077 -0.0060
33. (1.95720) BD ( 1) B  15 - C  16
            ( 33.95%)   0.5827* B  15 s( 37.77%)p 1.65( 62.19%)d 0.00(  0.04%)
                                    -0.0012  0.6145  0.0018  0.0069  0.0010
                                    -0.5565  0.0034 -0.0173 -0.3990  0.0015
                                    -0.0123  0.3904  0.0032  0.0120  0.0138
                                    -0.0106 -0.0073  0.0053 -0.0034
            ( 66.05%)   0.8127* C  16 s( 46.89%)p 1.13( 53.11%)d 0.00(  0.01%)
                                     0.0000  0.6845 -0.0171 -0.0050  0.0001
                                     0.5370 -0.0245 -0.0049  0.4029 -0.0194
                                    -0.0035 -0.2812  0.0163  0.0008  0.0037
                                    -0.0034 -0.0045  0.0027 -0.0010
34. (1.97511) BD ( 1) C  16 - N  17
            ( 37.05%)   0.6087* C  16 s( 26.30%)p 2.80( 73.63%)d 0.00(  0.07%)
                                    -0.0004  0.5122  0.0236  0.0037 -0.0003
                                    -0.8032 -0.0162 -0.0108 -0.0083  0.0092
                                     0.0049 -0.3003 -0.0176 -0.0091  0.0067
                                     0.0107  0.0011  0.0214 -0.0115
            ( 62.95%)   0.7934* N  17 s( 34.38%)p 1.91( 65.56%)d 0.00(  0.06%)
                                    -0.0001  0.5864 -0.0022 -0.0015  0.0001
                                     0.7863 -0.0066 -0.0019  0.0549 -0.0116
                                     0.0031  0.1846  0.0087 -0.0045  0.0012
                                     0.0131 -0.0012  0.0179 -0.0081
35. (1.85625) BD ( 2) C  16 - N  17
            ( 25.94%)   0.5093* C  16 s(  0.07%)p99.99( 99.77%)d 2.47(  0.16%)
                                     0.0001  0.0253  0.0036 -0.0009  0.0004
                                    -0.2338 -0.0032 -0.0016  0.7218  0.0263
                                    -0.0108  0.6489  0.0149 -0.0030 -0.0258
                                    -0.0251 -0.0090  0.0145 -0.0061
            ( 74.06%)   0.8606* N  17 s(  0.02%)p99.99( 99.96%)d 0.83(  0.02%)
                                     0.0000 -0.0143  0.0040 -0.0006  0.0000
                                    -0.1986 -0.0038 -0.0022  0.7039  0.0040
                                     0.0076  0.6816  0.0057  0.0065  0.0077
                                     0.0049  0.0034  0.0004  0.0094
36. (1.97558) BD ( 1) C  16 - N  20
            ( 37.02%)   0.6085* C  16 s( 26.80%)p 2.73( 73.13%)d 0.00(  0.07%)
                                    -0.0003  0.5170  0.0259  0.0042 -0.0001
                                     0.0963  0.0178  0.0088 -0.5605 -0.0103
                                    -0.0076  0.6379  0.0143  0.0130  0.0019
                                    -0.0022 -0.0231 -0.0113  0.0068
            ( 62.98%)   0.7936* N  20 s( 34.60%)p 1.89( 65.35%)d 0.00(  0.05%)
                                    -0.0001  0.5882 -0.0036 -0.0020  0.0001
                                     0.0229 -0.0153  0.0047  0.5448 -0.0081
                                    -0.0012 -0.5965  0.0009  0.0033 -0.0013
                                     0.0028 -0.0204 -0.0079  0.0071
37. (1.97731) BD ( 1) N  17 - C  18
            ( 61.94%)   0.7870* N  17 s( 31.37%)p 2.19( 68.57%)d 0.00(  0.05%)
                                    -0.0001  0.5601 -0.0057  0.0000  0.0001
                                    -0.4787  0.0226 -0.0035 -0.5294  0.0078
                                     0.0015  0.4191  0.0062 -0.0032  0.0129
                                    -0.0110 -0.0158 -0.0027 -0.0006
            ( 38.06%)   0.6169* C  18 s( 28.59%)p 2.50( 71.35%)d 0.00(  0.07%)
                                    -0.0001  0.5346  0.0044  0.0015 -0.0011
                                     0.3761 -0.0019 -0.0064  0.5764  0.0225
                                     0.0011 -0.4884 -0.0260 -0.0067  0.0166
                                    -0.0107 -0.0163  0.0000 -0.0038
38. (1.98138) BD ( 1) N  17 - C  21
            ( 63.11%)   0.7944* N  17 s( 34.18%)p 1.92( 65.78%)d 0.00(  0.03%)
                                    -0.0001  0.5846  0.0029  0.0013 -0.0001
                                    -0.3348 -0.0051  0.0045  0.4695  0.0027
                                    -0.0052 -0.5702 -0.0066  0.0070 -0.0074
                                     0.0091 -0.0141 -0.0023  0.0024
            ( 36.89%)   0.6074* C  21 s( 25.90%)p 2.86( 74.02%)d 0.00(  0.07%)
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                                    -0.0002  0.5088  0.0080  0.0075 -0.0006
                                     0.3843  0.0033  0.0051 -0.5020  0.0002
                                    -0.0066  0.5834  0.0058  0.0075 -0.0121
                                     0.0132 -0.0184 -0.0049  0.0059
39. (1.97697) BD ( 1) C  18 - C  19
            ( 49.97%)   0.7069* C  18 s( 37.04%)p 1.70( 62.91%)d 0.00(  0.05%)
                                     0.0000 -0.6085 -0.0095 -0.0027 -0.0007
                                    -0.4291  0.0111  0.0143  0.3778  0.0241
                                     0.0094 -0.5484 -0.0219 -0.0041  0.0081
                                    -0.0167  0.0116 -0.0080 -0.0012
            ( 50.03%)   0.7073* C  19 s( 37.19%)p 1.69( 62.76%)d 0.00(  0.05%)
                                     0.0000 -0.6097 -0.0092 -0.0028 -0.0006
                                     0.5697  0.0334  0.0103 -0.2598  0.0086
                                     0.0130  0.4838  0.0013 -0.0070  0.0083
                                    -0.0153  0.0146 -0.0040 -0.0036
40. (1.87142) BD ( 2) C  18 - C  19
            ( 49.67%)   0.7047* C  18 s(  0.00%)p 1.00( 99.94%)d 0.00(  0.06%)
                                     0.0000  0.0007 -0.0023  0.0012  0.0001
                                    -0.2259  0.0043  0.0000  0.7106 -0.0159
                                     0.0003  0.6655 -0.0144  0.0008  0.0156
                                     0.0102  0.0056 -0.0009  0.0149
            ( 50.33%)   0.7095* C  19 s(  0.00%)p 1.00( 99.94%)d 0.00(  0.06%)
                                     0.0000  0.0027 -0.0028  0.0019  0.0001
                                    -0.2352  0.0051 -0.0005  0.7109 -0.0170
                                     0.0014  0.6620 -0.0139  0.0000 -0.0099
                                    -0.0021 -0.0036 -0.0074 -0.0203
41. (1.97977) BD ( 1) C  18 - H  63
            ( 62.20%)   0.7886* C  18 s( 34.32%)p 1.91( 65.66%)d 0.00(  0.02%)
                                     0.0003 -0.5857  0.0077  0.0033 -0.0002
                                     0.7890 -0.0146  0.0005  0.1341 -0.0003
                                     0.0085  0.1252 -0.0058 -0.0082 -0.0036
                                    -0.0043  0.0000 -0.0120  0.0068
            ( 37.80%)   0.6148* H  63 s( 99.93%)p 0.00(  0.07%)
                                    -0.9997 -0.0018 -0.0002 -0.0252 -0.0037
                                    -0.0045
42. (1.97686) BD ( 1) C  19 - N  20
            ( 37.98%)   0.6163* C  19 s( 28.42%)p 2.52( 71.51%)d 0.00(  0.07%)
                                    -0.0001  0.5331  0.0043  0.0013 -0.0012
                                     0.7774  0.0331  0.0053  0.3228  0.0004
                                    -0.0070 -0.0726  0.0095  0.0051  0.0178
                                    -0.0061 -0.0073  0.0116 -0.0109
            ( 62.02%)   0.7875* N  20 s( 31.27%)p 2.20( 68.68%)d 0.00(  0.05%)
                                    -0.0001  0.5592 -0.0037  0.0003  0.0001
                                    -0.7108  0.0036  0.0032 -0.3916  0.0201
                                    -0.0033  0.1659 -0.0141  0.0029  0.0148
                                    -0.0045 -0.0036  0.0134 -0.0104
43. (1.98034) BD ( 1) C  19 - H  64
            ( 62.13%)   0.7882* C  19 s( 34.33%)p 1.91( 65.65%)d 0.00(  0.02%)
                                     0.0003 -0.5858  0.0073  0.0033 -0.0002
                                     0.1129  0.0021  0.0106  0.5674 -0.0108
                                     0.0028 -0.5669  0.0110  0.0037 -0.0022
                                     0.0018  0.0130  0.0057 -0.0036
            ( 37.87%)   0.6154* H  64 s( 99.93%)p 0.00(  0.07%)
                                    -0.9997 -0.0019 -0.0002 -0.0030 -0.0183
                                     0.0182
44. (1.98185) BD ( 1) N  20 - C  31
            ( 62.78%)   0.7923* N  20 s( 34.08%)p 1.93( 65.89%)d 0.00(  0.04%)
                                    -0.0001  0.5838  0.0027  0.0017 -0.0002
                                     0.6545  0.0049 -0.0078 -0.1638 -0.0043
                                     0.0023  0.4511  0.0052 -0.0056 -0.0032
                                     0.0152 -0.0046  0.0103  0.0002
            ( 37.22%)   0.6101* C  31 s( 26.18%)p 2.82( 73.75%)d 0.00(  0.07%)
                                    -0.0002  0.5116  0.0082  0.0071 -0.0004
                                    -0.6697 -0.0030 -0.0076  0.1648  0.0037
                                     0.0014 -0.5115 -0.0015 -0.0063 -0.0069
                                     0.0213 -0.0037  0.0136  0.0005
45. (1.96835) BD ( 1) C  21 - C  22
            ( 50.89%)   0.7133* C  21 s( 37.14%)p 1.69( 62.82%)d 0.00(  0.05%)
                                    -0.0002  0.6094 -0.0012 -0.0033  0.0001
                                     0.0162 -0.0063 -0.0045 -0.2457  0.0018
                                    -0.0007 -0.7533 -0.0054  0.0006 -0.0014
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                                     0.0002  0.0119 -0.0035  0.0176
            ( 49.11%)   0.7008* C  22 s( 33.53%)p 1.98( 66.42%)d 0.00(  0.06%)
                                     0.0000  0.5790  0.0030 -0.0011  0.0000
                                     0.0120 -0.0097 -0.0007  0.2101  0.0098
                                    -0.0023  0.7872  0.0007  0.0016 -0.0018
                                    -0.0009  0.0108 -0.0026  0.0206
46. (1.96787) BD ( 1) C  21 - C  26
            ( 50.49%)   0.7105* C  21 s( 36.89%)p 1.71( 63.07%)d 0.00(  0.05%)
                                    -0.0002  0.6073 -0.0019 -0.0025  0.0002
                                    -0.3615 -0.0084 -0.0040  0.6531  0.0045
                                     0.0017  0.2708 -0.0021  0.0000 -0.0152
                                    -0.0061  0.0106 -0.0082 -0.0049
            ( 49.51%)   0.7036* C  26 s( 34.11%)p 1.93( 65.83%)d 0.00(  0.05%)
                                     0.0000  0.5841  0.0031 -0.0005  0.0000
                                     0.3858 -0.0048 -0.0013 -0.6772 -0.0003
                                    -0.0011 -0.2253 -0.0121  0.0031 -0.0157
                                    -0.0053  0.0105 -0.0099 -0.0063
47. (1.67376) BD ( 2) C  21 - C  26
            ( 53.97%)   0.7346* C  21 s(  0.04%)p99.99( 99.94%)d 0.56(  0.02%)
                                     0.0002  0.0165  0.0091 -0.0003 -0.0003
                                     0.8489 -0.0014 -0.0054  0.5104 -0.0067
                                    -0.0051 -0.1348  0.0024  0.0031  0.0047
                                     0.0029 -0.0004 -0.0130  0.0003
            ( 46.03%)   0.6785* C  26 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                     0.0000  0.0009  0.0057 -0.0020 -0.0002
                                     0.8387 -0.0097 -0.0036  0.5255 -0.0027
                                     0.0014 -0.1409  0.0020  0.0018 -0.0098
                                    -0.0126 -0.0052  0.0135  0.0036
48. (1.97239) BD ( 1) C  22 - C  23
            ( 50.45%)   0.7103* C  22 s( 34.21%)p 1.92( 65.75%)d 0.00(  0.05%)
                                    -0.0001  0.5848  0.0089  0.0043  0.0003
                                    -0.3818 -0.0038 -0.0048  0.4604  0.0050
                                    -0.0007 -0.5473  0.0078 -0.0115 -0.0122
                                     0.0121 -0.0123 -0.0026  0.0031
            ( 49.55%)   0.7039* C  23 s( 35.86%)p 1.79( 64.08%)d 0.00(  0.06%)
                                     0.0001  0.5988 -0.0004 -0.0041 -0.0003
                                     0.3862  0.0115 -0.0045 -0.4769 -0.0167
                                     0.0050  0.5135 -0.0026 -0.0092 -0.0134
                                     0.0132 -0.0150 -0.0037  0.0054
49. (1.63022) BD ( 2) C  22 - C  23
            ( 48.31%)   0.6950* C  22 s(  0.02%)p99.99( 99.94%)d 1.71(  0.03%)
                                    -0.0002 -0.0062 -0.0128  0.0010  0.0006
                                    -0.8456  0.0042 -0.0024 -0.5105  0.0073
                                     0.0028  0.1537 -0.0064 -0.0038 -0.0065
                                     0.0004  0.0033  0.0172 -0.0010
            ( 51.69%)   0.7190* C  23 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.03%)
                                     0.0000 -0.0001 -0.0045  0.0001  0.0001
                                    -0.8394  0.0021 -0.0147 -0.5229  0.0037
                                    -0.0117  0.1459  0.0003  0.0029  0.0013
                                    -0.0134 -0.0097 -0.0065  0.0038
50. (1.96962) BD ( 1) C  22 - C  27
            ( 50.20%)   0.7085* C  22 s( 32.22%)p 2.10( 67.75%)d 0.00(  0.03%)
                                    -0.0001  0.5676 -0.0058 -0.0042 -0.0003
                                     0.3719  0.0040 -0.0033 -0.6945 -0.0166
                                     0.0064 -0.2375 -0.0045 -0.0009 -0.0117
                                    -0.0025  0.0067 -0.0096 -0.0059
            ( 49.80%)   0.7057* C  27 s( 26.68%)p 2.75( 73.27%)d 0.00(  0.06%)
                                     0.0001  0.5165  0.0001 -0.0014  0.0005
                                    -0.3744  0.0052  0.0001  0.7310  0.0012
                                    -0.0007  0.2409  0.0001 -0.0030 -0.0156
                                    -0.0057  0.0105 -0.0102 -0.0090
51. (1.98062) BD ( 1) C  23 - C  24
            ( 50.11%)   0.7079* C  23 s( 35.87%)p 1.79( 64.07%)d 0.00(  0.05%)
                                     0.0000  0.5988  0.0135  0.0054  0.0002
                                    -0.3811 -0.0137 -0.0036  0.6705  0.0165
                                     0.0022  0.2117 -0.0198 -0.0137 -0.0142
                                    -0.0065  0.0133 -0.0091 -0.0040
            ( 49.89%)   0.7064* C  24 s( 35.96%)p 1.78( 63.97%)d 0.00(  0.07%)
                                     0.0000  0.5996  0.0058 -0.0020 -0.0002
                                     0.3654  0.0027 -0.0084 -0.6618 -0.0113
                                     0.0099 -0.2588 -0.0295 -0.0077 -0.0197
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                                    -0.0032  0.0067 -0.0111 -0.0102
52. (1.97434) BD ( 1) C  23 - H  67
            ( 61.07%)   0.7815* C  23 s( 28.23%)p 2.54( 71.73%)d 0.00(  0.04%)
                                     0.0004 -0.5312  0.0109  0.0014 -0.0001
                                     0.0058 -0.0002  0.0024  0.2188 -0.0095
                                    -0.0046  0.8179 -0.0147 -0.0124  0.0002
                                    -0.0002 -0.0087  0.0015 -0.0168
            ( 38.93%)   0.6239* H  67 s( 99.94%)p 0.00(  0.06%)
                                    -0.9997  0.0017 -0.0014  0.0015 -0.0058
                                    -0.0227
53. (1.98089) BD ( 1) C  24 - C  25
            ( 49.76%)   0.7054* C  24 s( 35.96%)p 1.78( 63.97%)d 0.00(  0.07%)
                                     0.0000 -0.5996 -0.0080  0.0020  0.0001
                                     0.0142  0.0136  0.0068 -0.2360 -0.0263
                                    -0.0060 -0.7633 -0.0136  0.0116  0.0014
                                    -0.0031 -0.0075  0.0015 -0.0243
            ( 50.24%)   0.7088* C  25 s( 36.10%)p 1.77( 63.85%)d 0.00(  0.05%)
                                     0.0000 -0.6007 -0.0144 -0.0044 -0.0001
                                     0.0185  0.0138  0.0087  0.1930 -0.0170
                                    -0.0104  0.7744  0.0202  0.0033  0.0022
                                     0.0021 -0.0135  0.0033 -0.0176
54. (1.66929) BD ( 2) C  24 - C  25
            ( 48.85%)   0.6989* C  24 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                     0.0000  0.0002  0.0031 -0.0021  0.0001
                                     0.8406 -0.0071  0.0095  0.5212 -0.0042
                                     0.0054 -0.1457  0.0013 -0.0018  0.0007
                                     0.0125  0.0084  0.0044 -0.0043
            ( 51.15%)   0.7152* C  25 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                                     0.0001  0.0006  0.0011 -0.0012 -0.0003
                                     0.8397 -0.0082  0.0181  0.5214 -0.0050
                                     0.0106 -0.1495 -0.0003 -0.0033 -0.0059
                                    -0.0092 -0.0038  0.0092  0.0025
55. (1.97747) BD ( 1) C  24 - H  66
            ( 60.90%)   0.7804* C  24 s( 28.03%)p 2.57( 71.94%)d 0.00(  0.03%)
                                    -0.0004  0.5293 -0.0115  0.0035  0.0003
                                    -0.3984  0.0123 -0.0025  0.4827 -0.0132
                                     0.0020 -0.5719  0.0153 -0.0022 -0.0045
                                     0.0098 -0.0143  0.0006  0.0005
            ( 39.10%)   0.6253* H  66 s( 99.95%)p 0.00(  0.05%)
                                     0.9997  0.0014  0.0005  0.0106 -0.0132
                                     0.0158
56. (1.97185) BD ( 1) C  25 - C  26
            ( 49.37%)   0.7026* C  25 s( 35.74%)p 1.80( 64.20%)d 0.00(  0.06%)
                                     0.0001  0.5978 -0.0017 -0.0044 -0.0001
                                     0.3694  0.0031 -0.0060 -0.4342  0.0022
                                     0.0071  0.5626  0.0199 -0.0057 -0.0129
                                     0.0134 -0.0148 -0.0033  0.0060
            ( 50.63%)   0.7116* C  26 s( 33.98%)p 1.94( 65.97%)d 0.00(  0.05%)
                                    -0.0002  0.5828  0.0099  0.0029  0.0001
                                    -0.3836  0.0037 -0.0077  0.4652 -0.0079
                                     0.0077 -0.5441 -0.0034  0.0000 -0.0110
                                     0.0119 -0.0127 -0.0023  0.0058
57. (1.97514) BD ( 1) C  25 - H  65
            ( 60.81%)   0.7798* C  25 s( 28.12%)p 2.55( 71.84%)d 0.00(  0.04%)
                                    -0.0004  0.5302 -0.0105 -0.0004  0.0001
                                    -0.3966  0.0066  0.0044  0.7080 -0.0112
                                    -0.0105  0.2439 -0.0108 -0.0055 -0.0129
                                    -0.0046  0.0083 -0.0079 -0.0066
            ( 39.19%)   0.6260* H  65 s( 99.95%)p 0.00(  0.05%)
                                     0.9997  0.0020  0.0013  0.0105 -0.0195
                                    -0.0069
58. (1.96965) BD ( 1) C  26 - C  29
            ( 50.05%)   0.7075* C  26 s( 31.88%)p 2.14( 68.09%)d 0.00(  0.03%)
                                    -0.0001  0.5645 -0.0074 -0.0031 -0.0002
                                    -0.0045 -0.0027 -0.0007  0.2195  0.0065
                                    -0.0004  0.7952  0.0162 -0.0049 -0.0013
                                     0.0000  0.0072 -0.0015  0.0161
            ( 49.95%)   0.7068* C  29 s( 26.68%)p 2.75( 73.27%)d 0.00(  0.06%)
                                     0.0001  0.5165  0.0016 -0.0017 -0.0001
                                     0.0141  0.0025 -0.0022 -0.2394 -0.0010
                                     0.0018 -0.8217  0.0018  0.0030 -0.0001
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                                    -0.0005  0.0113 -0.0015  0.0206
59. (1.97151) BD ( 1) C  27 - C  28
            ( 50.49%)   0.7105* C  27 s( 25.54%)p 2.91( 74.42%)d 0.00(  0.04%)
                                    -0.0001  0.5053 -0.0112  0.0022 -0.0001
                                    -0.5593  0.0005 -0.0003 -0.6556 -0.0122
                                    -0.0041  0.0376  0.0039  0.0008  0.0172
                                    -0.0017 -0.0010 -0.0006 -0.0104
            ( 49.51%)   0.7037* C  28 s( 29.27%)p 2.41( 70.68%)d 0.00(  0.04%)
                                     0.0004  0.5407 -0.0193 -0.0030  0.0001
                                     0.5458  0.0107 -0.0077  0.6389  0.0071
                                    -0.0132 -0.0176 -0.0006  0.0013  0.0179
                                    -0.0005 -0.0007 -0.0031 -0.0107
60. (1.97918) BD ( 1) C  27 - C  62
            ( 51.43%)   0.7172* C  27 s( 26.93%)p 2.71( 73.03%)d 0.00(  0.04%)
                                     0.0001 -0.5188  0.0115 -0.0033  0.0002
                                    -0.3401 -0.0136 -0.0031 -0.0651  0.0020
                                     0.0012  0.7811 -0.0053  0.0039 -0.0016
                                     0.0112  0.0022 -0.0017 -0.0153
            ( 48.57%)   0.6969* C  62 s( 28.50%)p 2.51( 71.45%)d 0.00(  0.05%)
                                    -0.0003 -0.5334  0.0218  0.0029  0.0000
                                     0.3602  0.0039 -0.0095  0.0533  0.0064
                                    -0.0003 -0.7625 -0.0130  0.0123 -0.0009
                                     0.0153  0.0027 -0.0038 -0.0157
61. (1.95937) BD ( 1) C  27 - H  84
            ( 61.62%)   0.7850* C  27 s( 20.90%)p 3.78( 79.05%)d 0.00(  0.05%)
                                    -0.0002  0.4567  0.0204 -0.0043 -0.0001
                                     0.6559 -0.0047 -0.0021 -0.1755  0.0063
                                    -0.0063  0.5737 -0.0132 -0.0056 -0.0050
                                     0.0190 -0.0051  0.0092  0.0039
            ( 38.38%)   0.6195* H  84 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0050  0.0007 -0.0169  0.0024
                                    -0.0125
62. (1.98583) BD ( 1) C  28 - H  90
            ( 60.77%)   0.7795* C  28 s( 23.20%)p 3.31( 76.76%)d 0.00(  0.04%)
                                     0.0002 -0.4816 -0.0056 -0.0024 -0.0001
                                    -0.3911  0.0046  0.0039  0.7480 -0.0050
                                     0.0078  0.2347 -0.0020 -0.0009  0.0144
                                     0.0042 -0.0079  0.0098  0.0076
            ( 39.23%)   0.6264* H  90 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0016 -0.0002  0.0112 -0.0159
                                    -0.0062
63. (1.98733) BD ( 1) C  28 - H  91
            ( 60.46%)   0.7776* C  28 s( 23.87%)p 3.19( 76.08%)d 0.00(  0.05%)
                                     0.0000 -0.4885 -0.0040 -0.0014  0.0001
                                     0.3302 -0.0010  0.0058  0.1091  0.0013
                                     0.0084 -0.7999  0.0030  0.0005  0.0004
                                     0.0132  0.0049 -0.0032 -0.0169
            ( 39.54%)   0.6288* H  91 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0016  0.0000 -0.0060 -0.0017
                                     0.0197
64. (1.98896) BD ( 1) C  28 - H  92
            ( 60.68%)   0.7790* C  28 s( 23.66%)p 3.23( 76.30%)d 0.00(  0.05%)
                                     0.0000 -0.4863 -0.0077  0.0005  0.0000
                                     0.6627  0.0002  0.0075 -0.1397  0.0033
                                     0.0065  0.5516 -0.0033  0.0004  0.0055
                                    -0.0170  0.0029 -0.0109 -0.0023
            ( 39.32%)   0.6270* H  92 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0023 -0.0002 -0.0155  0.0051
                                    -0.0144
65. (1.97625) BD ( 1) C  29 - C  30
            ( 50.69%)   0.7120* C  29 s( 26.01%)p 2.84( 73.95%)d 0.00(  0.04%)
                                    -0.0001  0.5098 -0.0125  0.0007  0.0000
                                    -0.8057 -0.0033 -0.0026  0.0250 -0.0086
                                     0.0004  0.2992  0.0115  0.0030 -0.0012
                                    -0.0098  0.0003  0.0155 -0.0063
            ( 49.31%)   0.7022* C  30 s( 29.30%)p 2.41( 70.65%)d 0.00(  0.05%)
                                     0.0003  0.5410 -0.0190 -0.0027  0.0001
                                     0.7841  0.0125 -0.0134 -0.0260 -0.0014
                                    -0.0007 -0.3011 -0.0002  0.0070 -0.0006
                                    -0.0124  0.0001  0.0161 -0.0065
66. (1.97478) BD ( 1) C  29 - C  61
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           ( 51.28%)   0.7161* C  29 s( 26.46%)p 2.78( 73.50%)d 0.00(  0.04%)
                                     -0.0001  0.5143 -0.0111  0.0012  0.0001
                                      0.3898  0.0116  0.0009  0.7555 -0.0018
                                      0.0055  0.1098  0.0075  0.0042  0.0130
                                      0.0013  0.0030 -0.0098 -0.0089
           ( 48.72%)   0.6980* C  61 s( 28.85%)p 2.46( 71.10%)d 0.00(  0.05%)
                                      0.0003  0.5370 -0.0135  0.0007 -0.0005
                                     -0.3908 -0.0054  0.0080 -0.7377 -0.0078
                                      0.0073 -0.1179  0.0041  0.0017  0.0154
                                      0.0026  0.0043 -0.0098 -0.0100
67. (1.96477) BD ( 1) C  29 - H  83
           ( 61.05%)   0.7813* C  29 s( 20.90%)p 3.78( 79.05%)d 0.00(  0.05%)
                                     -0.0002  0.4567  0.0201 -0.0004  0.0001
                                      0.4447 -0.0057 -0.0051 -0.6083  0.0122
                                      0.0052  0.4717 -0.0062  0.0050 -0.0137
                                      0.0105 -0.0147 -0.0046 -0.0018
           ( 38.95%)   0.6241* H  83 s( 99.96%)p 0.00(  0.04%)
                                      0.9998  0.0054  0.0001 -0.0113  0.0145
                                     -0.0104
68. (1.98638) BD ( 1) C  30 - H  93
           ( 60.74%)   0.7794* C  30 s( 23.29%)p 3.29( 76.67%)d 0.00(  0.04%)
                                     -0.0001  0.4826  0.0052  0.0019  0.0002
                                      0.0011 -0.0026 -0.0077  0.2021 -0.0017
                                     -0.0005  0.8519 -0.0056  0.0047  0.0000
                                      0.0001  0.0081 -0.0019  0.0193
           ( 39.26%)   0.6265* H  93 s( 99.96%)p 0.00(  0.04%)
                                      0.9998  0.0015  0.0002 -0.0020 -0.0050
                                     -0.0203
69. (1.98825) BD ( 1) C  30 - H  94
           ( 60.66%)   0.7789* C  30 s( 23.75%)p 3.21( 76.20%)d 0.00(  0.05%)
                                      0.0000  0.4873  0.0067 -0.0002 -0.0001
                                     -0.4764 -0.0046 -0.0087  0.6003 -0.0031
                                      0.0010 -0.4178  0.0031  0.0025 -0.0138
                                      0.0106 -0.0112 -0.0039 -0.0031
           ( 39.34%)   0.6272* H  94 s( 99.95%)p 0.00(  0.05%)
                                      0.9998  0.0022  0.0002  0.0107 -0.0148
                                      0.0113
70. (1.98830) BD ( 1) C  30 - H  95
           ( 60.73%)   0.7793* C  30 s( 23.66%)p 3.22( 76.29%)d 0.00(  0.05%)
                                     -0.0001  0.4864  0.0049  0.0014 -0.0001
                                     -0.3962 -0.0009 -0.0082 -0.7729  0.0056
                                     -0.0006 -0.0916  0.0009  0.0042  0.0150
                                      0.0031  0.0031 -0.0112 -0.0091
           ( 39.27%)   0.6267* H  95 s( 99.96%)p 0.00(  0.04%)
                                      0.9998  0.0012  0.0001  0.0092  0.0184
                                      0.0025
71. (1.96778) BD ( 1) C  31 - C  32
           ( 50.61%)   0.7114* C  31 s( 36.78%)p 1.72( 63.17%)d 0.00(  0.05%)
                                     -0.0002  0.6065 -0.0017 -0.0032  0.0001
                                      0.0389  0.0034  0.0005  0.4016 -0.0020
                                     -0.0015  0.6847  0.0088  0.0028 -0.0012
                                      0.0011  0.0166 -0.0036  0.0135
           ( 49.39%)   0.7028* C  32 s( 33.82%)p 1.96( 66.13%)d 0.00(  0.05%)
                                      0.0000  0.5815  0.0025 -0.0007  0.0000
                                     -0.0788  0.0101 -0.0023 -0.3802 -0.0088
                                      0.0001 -0.7143  0.0021  0.0014 -0.0004
                                      0.0025  0.0176 -0.0042  0.0140
72. (1.96880) BD ( 1) C  31 - C  36
           ( 50.73%)   0.7122* C  31 s( 36.98%)p 1.70( 62.97%)d 0.00(  0.05%)
                                     -0.0002  0.6081 -0.0016 -0.0025  0.0001
                                      0.5173  0.0061  0.0000 -0.5489 -0.0054
                                     -0.0031 -0.2464  0.0054  0.0025 -0.0169
                                     -0.0061  0.0095 -0.0022 -0.0070
           ( 49.27%)   0.7020* C  36 s( 33.78%)p 1.96( 66.16%)d 0.00(  0.05%)
                                      0.0000  0.5812  0.0025 -0.0001  0.0000
                                     -0.5450  0.0036 -0.0022  0.5690  0.0023
                                     -0.0011  0.2015  0.0133 -0.0006 -0.0186
                                     -0.0066  0.0093 -0.0008 -0.0077
73. (1.65932) BD ( 2) C  31 - C  36
           ( 54.31%)   0.7370* C  31 s(  0.01%)p99.99( 99.97%)d 1.31(  0.02%)
                                      0.0002  0.0082  0.0087 -0.0009 -0.0001
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                                     0.5306 -0.0061 -0.0063  0.7140 -0.0026
                                    -0.0042 -0.4562  0.0007  0.0033  0.0013
                                    -0.0047  0.0046  0.0119  0.0012
            ( 45.69%)   0.6759* C  36 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                     0.0000  0.0004  0.0057 -0.0010 -0.0001
                                     0.5517 -0.0041  0.0008  0.6923 -0.0101
                                    -0.0043 -0.4644  0.0046  0.0005  0.0017
                                     0.0118  0.0024 -0.0155 -0.0107
74. (1.97272) BD ( 1) C  32 - C  33
            ( 50.56%)   0.7110* C  32 s( 34.05%)p 1.94( 65.90%)d 0.00(  0.05%)
                                    -0.0001  0.5834  0.0094  0.0040  0.0001
                                     0.6245  0.0001  0.0038 -0.1621 -0.0065
                                     0.0023  0.4925 -0.0078  0.0093 -0.0081
                                     0.0169 -0.0031  0.0103  0.0005
            ( 49.44%)   0.7032* C  33 s( 35.75%)p 1.80( 64.19%)d 0.00(  0.06%)
                                     0.0001  0.5979 -0.0011 -0.0044 -0.0001
                                    -0.6298 -0.0154  0.0076  0.1843  0.0134
                                    -0.0007 -0.4591  0.0018  0.0081 -0.0085
                                     0.0198 -0.0030  0.0117  0.0013
75. (1.64228) BD ( 2) C  32 - C  33
            ( 48.38%)   0.6956* C  32 s(  0.01%)p 1.00( 99.96%)d 0.00(  0.03%)
                                     0.0001  0.0002  0.0071 -0.0021 -0.0001
                                     0.5350 -0.0046 -0.0012  0.7197 -0.0022
                                     0.0042 -0.4419  0.0039  0.0014  0.0053
                                    -0.0052  0.0062  0.0150 -0.0017
            ( 51.62%)   0.7184* C  33 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                     0.0001  0.0016  0.0012 -0.0001 -0.0001
                                     0.5376 -0.0028  0.0092  0.7132 -0.0032
                                     0.0113 -0.4491  0.0015 -0.0089 -0.0083
                                    -0.0035 -0.0097 -0.0037  0.0113
76. (1.97001) BD ( 1) C  32 - C  37
            ( 50.23%)   0.7087* C  32 s( 32.10%)p 2.11( 67.87%)d 0.00(  0.03%)
                                    -0.0001  0.5665 -0.0064 -0.0038  0.0000
                                    -0.5628 -0.0103  0.0042  0.5572  0.0122
                                    -0.0048  0.2264  0.0063 -0.0002 -0.0144
                                    -0.0047  0.0061  0.0010 -0.0064
            ( 49.77%)   0.7055* C  37 s( 26.54%)p 2.77( 73.40%)d 0.00(  0.06%)
                                     0.0001  0.5152  0.0012 -0.0021 -0.0001
                                     0.5819 -0.0019 -0.0024 -0.5808  0.0006
                                     0.0011 -0.2409 -0.0016  0.0035 -0.0189
                                    -0.0080  0.0079 -0.0002 -0.0090
77. (1.98090) BD ( 1) C  33 - C  34
            ( 50.22%)   0.7086* C  33 s( 36.06%)p 1.77( 63.89%)d 0.00(  0.05%)
                                     0.0000  0.6003  0.0142  0.0045  0.0000
                                     0.5534  0.0226  0.0069 -0.5416 -0.0063
                                     0.0020 -0.1955  0.0178  0.0118 -0.0170
                                    -0.0080  0.0113 -0.0022 -0.0056
            ( 49.78%)   0.7056* C  34 s( 35.89%)p 1.78( 64.04%)d 0.00(  0.07%)
                                     0.0000  0.5990  0.0074 -0.0018 -0.0001
                                    -0.5213  0.0002  0.0098  0.5587  0.0181
                                    -0.0052  0.2351  0.0270  0.0075 -0.0221
                                    -0.0044  0.0059  0.0021 -0.0108
78. (1.97515) BD ( 1) C  33 - H  70
            ( 60.92%)   0.7805* C  33 s( 28.16%)p 2.55( 71.80%)d 0.00(  0.04%)
                                    -0.0004  0.5306 -0.0109 -0.0005  0.0001
                                     0.0816  0.0035  0.0002  0.4036 -0.0098
                                    -0.0078  0.7403 -0.0129 -0.0104  0.0010
                                     0.0026  0.0140 -0.0038  0.0120
            ( 39.08%)   0.6251* H  70 s( 99.95%)p 0.00(  0.05%)
                                     0.9997  0.0019  0.0013 -0.0021 -0.0114
                                    -0.0202
79. (1.98086) BD ( 1) C  34 - C  35
            ( 49.88%)   0.7062* C  34 s( 36.02%)p 1.77( 63.92%)d 0.00(  0.06%)
                                     0.0000  0.6001  0.0067 -0.0022 -0.0002
                                    -0.0528  0.0196  0.0070 -0.4018 -0.0227
                                    -0.0036 -0.6883 -0.0117  0.0110  0.0021
                                     0.0078  0.0170 -0.0027  0.0169
            ( 50.12%)   0.7080* C  35 s( 35.99%)p 1.78( 63.96%)d 0.00(  0.05%)
                                     0.0000  0.5997  0.0141  0.0044  0.0001
                                     0.0989  0.0230  0.0088  0.3787 -0.0068
                                    -0.0087  0.6967  0.0182  0.0056 -0.0012
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                                    -0.0001  0.0182 -0.0056  0.0119
80. (1.66541) BD ( 2) C  34 - C  35
            ( 49.11%)   0.7008* C  34 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                     0.0000 -0.0020  0.0008 -0.0041 -0.0002
                                     0.5464 -0.0043  0.0015  0.7032 -0.0061
                                     0.0062 -0.4543  0.0042 -0.0038 -0.0066
                                    -0.0054 -0.0090 -0.0019  0.0108
            ( 50.89%)   0.7134* C  35 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.02%)
                                     0.0000 -0.0028 -0.0012 -0.0004 -0.0007
                                     0.5503 -0.0039  0.0071  0.6993 -0.0056
                                     0.0123 -0.4556  0.0037 -0.0088  0.0026
                                     0.0080  0.0007 -0.0107 -0.0078
81. (1.97730) BD ( 1) C  34 - H  69
            ( 61.01%)   0.7811* C  34 s( 28.04%)p 2.56( 71.92%)d 0.00(  0.03%)
                                    -0.0004  0.5294 -0.0119  0.0035  0.0003
                                     0.6523 -0.0173  0.0025 -0.1740  0.0054
                                    -0.0021  0.5127 -0.0149  0.0043 -0.0013
                                     0.0134 -0.0081  0.0086 -0.0004
            ( 38.99%)   0.6244* H  69 s( 99.95%)p 0.00(  0.05%)
                                     0.9997  0.0014  0.0005 -0.0178  0.0047
                                    -0.0142
82. (1.97274) BD ( 1) C  35 - C  36
            ( 49.43%)   0.7031* C  35 s( 35.77%)p 1.79( 64.16%)d 0.00(  0.06%)
                                     0.0001  0.5981 -0.0014 -0.0046 -0.0001
                                    -0.6018 -0.0037  0.0070  0.1453 -0.0067
                                    -0.0042 -0.5078 -0.0186  0.0049 -0.0082
                                     0.0202 -0.0033  0.0114  0.0020
            ( 50.57%)   0.7111* C  36 s( 34.00%)p 1.94( 65.95%)d 0.00(  0.05%)
                                    -0.0001  0.5830  0.0097  0.0032  0.0001
                                     0.6250 -0.0061  0.0075 -0.1702  0.0068
                                    -0.0074  0.4895  0.0045  0.0014 -0.0066
                                     0.0177 -0.0026  0.0094  0.0028
83. (1.97505) BD ( 1) C  35 - H  68
            ( 61.04%)   0.7813* C  35 s( 28.21%)p 2.54( 71.76%)d 0.00(  0.04%)
                                    -0.0004  0.5310 -0.0105 -0.0002  0.0001
                                     0.5693 -0.0071 -0.0068 -0.5878  0.0130
                                     0.0069 -0.2180  0.0083  0.0055 -0.0152
                                    -0.0057  0.0065 -0.0008 -0.0073
            ( 38.96%)   0.6242* H  68 s( 99.95%)p 0.00(  0.05%)
                                     0.9997 -0.0019  0.0015 -0.0154  0.0159
                                     0.0066
84. (1.96945) BD ( 1) C  36 - C  39
            ( 50.38%)   0.7098* C  36 s( 32.18%)p 2.11( 67.79%)d 0.00(  0.03%)
                                    -0.0001  0.5672 -0.0067 -0.0038 -0.0001
                                    -0.0846 -0.0002  0.0016 -0.4088 -0.0113
                                     0.0023 -0.7094 -0.0143  0.0049  0.0009
                                     0.0040  0.0133 -0.0031  0.0101
            ( 49.62%)   0.7044* C  39 s( 26.43%)p 2.78( 73.51%)d 0.00(  0.06%)
                                     0.0001  0.5141  0.0010 -0.0021 -0.0002
                                     0.0840 -0.0010  0.0001  0.4367  0.0029
                                    -0.0041  0.7330 -0.0018 -0.0024  0.0019
                                     0.0031  0.0177 -0.0054  0.0146
85. (1.97786) BD ( 1) C  37 - C  38
            ( 50.77%)   0.7125* C  37 s( 26.24%)p 2.81( 73.73%)d 0.00(  0.04%)
                                    -0.0001  0.5120 -0.0130  0.0007  0.0000
                                    -0.2983 -0.0144 -0.0026 -0.1711 -0.0027
                                     0.0009  0.7866  0.0000  0.0023  0.0018
                                    -0.0100 -0.0067  0.0012  0.0151
            ( 49.23%)   0.7017* C  38 s( 29.30%)p 2.41( 70.66%)d 0.00(  0.05%)
                                     0.0003  0.5409 -0.0191 -0.0022  0.0001
                                     0.3080  0.0004 -0.0074  0.1553  0.0041
                                    -0.0026 -0.7663 -0.0125  0.0130  0.0027
                                    -0.0126 -0.0067  0.0021  0.0157
86. (1.97252) BD ( 1) C  37 - C  55
            ( 51.43%)   0.7172* C  37 s( 26.40%)p 2.79( 73.56%)d 0.00(  0.03%)
                                    -0.0001  0.5137 -0.0103  0.0015  0.0001
                                     0.3214 -0.0052 -0.0016  0.7940  0.0075
                                     0.0068 -0.0400 -0.0084  0.0028  0.0118
                                    -0.0009 -0.0010 -0.0108 -0.0095
            ( 48.57%)   0.6969* C  55 s( 28.68%)p 2.48( 71.27%)d 0.00(  0.05%)
                                     0.0004  0.5354 -0.0131  0.0008 -0.0005
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                                    -0.3100 -0.0081  0.0025 -0.7838 -0.0066
                                     0.0090  0.0450  0.0031 -0.0042  0.0125
                                    -0.0009 -0.0026 -0.0133 -0.0107
 87. (1.96378) BD ( 1) C  37 - H  85
            ( 61.15%)   0.7820* C  37 s( 20.87%)p 3.79( 79.08%)d 0.00(  0.05%)
                                     0.0002 -0.4564 -0.0202  0.0004 -0.0001
                                     0.6842 -0.0102  0.0026  0.0463 -0.0035
                                    -0.0031  0.5659 -0.0096 -0.0078 -0.0018
                                    -0.0195 -0.0016 -0.0118 -0.0025
            ( 38.85%)   0.6233* H  85 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0055 -0.0003 -0.0160 -0.0013
                                    -0.0141
 88. (1.98608) BD ( 1) C  38 - H 105
            ( 60.86%)   0.7801* C  38 s( 23.26%)p 3.30( 76.70%)d 0.00(  0.04%)
                                    -0.0001  0.4823  0.0050  0.0014  0.0002
                                    -0.6347  0.0039 -0.0046  0.5690 -0.0053
                                    -0.0016  0.2004  0.0007  0.0077 -0.0169
                                    -0.0055  0.0062  0.0016 -0.0093
            ( 39.14%)   0.6256* H 105 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0013  0.0002  0.0151 -0.0144
                                    -0.0031
 89. (1.98876) BD ( 1) C  38 - H 106
            ( 60.83%)   0.7800* C  38 s( 23.69%)p 3.22( 76.26%)d 0.00(  0.04%)
                                    -0.0001  0.4867  0.0057  0.0014 -0.0001
                                    -0.3371  0.0018 -0.0046 -0.8043  0.0049
                                    -0.0022  0.0449  0.0034  0.0073  0.0122
                                     0.0001 -0.0020 -0.0124 -0.0117
            ( 39.17%)   0.6258* H 106 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0012  0.0001  0.0076  0.0195
                                    -0.0007
 90. (1.98837) BD ( 1) C  38 - H 107
            ( 60.57%)   0.7782* C  38 s( 23.75%)p 3.21( 76.20%)d 0.00(  0.05%)
                                     0.0000  0.4873  0.0061 -0.0002 -0.0001
                                     0.6228 -0.0046 -0.0024  0.0677 -0.0027
                                    -0.0014  0.6078  0.0039  0.0086  0.0015
                                     0.0190  0.0026  0.0083  0.0042
            ( 39.43%)   0.6280* H 107 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0023  0.0002 -0.0158 -0.0015
                                    -0.0142
 91. (1.97424) BD ( 1) C  39 - C  40
            ( 50.69%)   0.7120* C  39 s( 25.93%)p 2.85( 74.03%)d 0.00(  0.04%)
                                    -0.0001  0.5091 -0.0127  0.0008  0.0000
                                    -0.1679 -0.0122 -0.0013 -0.8291 -0.0066
                                    -0.0029  0.1563 -0.0056 -0.0017  0.0059
                                    -0.0010 -0.0074 -0.0154 -0.0076
            ( 49.31%)   0.7022* C  40 s( 29.25%)p 2.42( 70.71%)d 0.00(  0.05%)
                                     0.0003  0.5405 -0.0192 -0.0027  0.0001
                                     0.1631  0.0001 -0.0048  0.8120  0.0118
                                    -0.0144 -0.1443 -0.0058  0.0009  0.0074
                                    -0.0012 -0.0062 -0.0163 -0.0097
 92. (1.97484) BD ( 1) C  39 - C  56
            ( 51.57%)   0.7181* C  39 s( 26.76%)p 2.74( 73.21%)d 0.00(  0.03%)
                                    -0.0001  0.5172 -0.0107  0.0016  0.0001
                                     0.6945 -0.0043  0.0029  0.0842  0.0075
                                    -0.0041 -0.4924 -0.0115 -0.0055  0.0029
                                    -0.0144 -0.0013  0.0107 -0.0012
            ( 48.43%)   0.6959* C  56 s( 28.64%)p 2.49( 71.31%)d 0.00(  0.05%)
                                     0.0003  0.5350 -0.0137 -0.0009 -0.0005
                                    -0.6749 -0.0104  0.0077 -0.0911 -0.0043
                                     0.0040  0.4991  0.0006 -0.0072  0.0036
                                    -0.0176 -0.0028  0.0117  0.0006
 93. (1.96388) BD ( 1) C  39 - H  86
            ( 61.33%)   0.7831* C  39 s( 20.93%)p 3.78( 79.02%)d 0.00(  0.05%)
                                     0.0002 -0.4570 -0.0204  0.0005 -0.0001
                                     0.6937 -0.0148 -0.0011 -0.3371  0.0045
                                     0.0086  0.4416 -0.0045  0.0041  0.0119
                                    -0.0152  0.0071 -0.0093  0.0035
            ( 38.67%)   0.6218* H  86 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0050 -0.0003 -0.0161  0.0093
                                    -0.0107
 94. (1.98600) BD ( 1) C  40 - H  99
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            ( 60.87%)   0.7802* C  40 s( 23.33%)p 3.28( 76.62%)d 0.00(  0.04%)
                                      -0.0002  0.4830  0.0052  0.0020  0.0001
                                      -0.1246  0.0003 -0.0030 -0.4299  0.0014
                                      -0.0085 -0.7522  0.0064  0.0003  0.0022
                                       0.0044  0.0157 -0.0032  0.0126
            ( 39.13%)   0.6255* H  99 s( 99.96%)p 0.00(  0.04%)
                                       0.9998  0.0015  0.0002  0.0026  0.0085
                                       0.0190
 95. (1.98848) BD ( 1) C  40 - H 100
            ( 60.59%)   0.7784* C  40 s( 23.74%)p 3.21( 76.21%)d 0.00(  0.05%)
                                       0.0000  0.4872  0.0070 -0.0002 -0.0001
                                       0.6620 -0.0040 -0.0009 -0.3821 -0.0043
                                      -0.0090  0.4216  0.0002  0.0023 -0.0130
                                       0.0130 -0.0075  0.0076 -0.0021
            ( 39.41%)   0.6278* H 100 s( 99.95%)p 0.00(  0.05%)
                                       0.9998  0.0023  0.0002 -0.0169  0.0084
                                      -0.0106
 96. (1.98843) BD ( 1) C  40 - H 101
            ( 60.68%)   0.7790* C  40 s( 23.68%)p 3.22( 76.28%)d 0.00(  0.05%)
                                       0.0001 -0.4866 -0.0049 -0.0013  0.0001
                                       0.7204 -0.0044  0.0028  0.0929  0.0021
                                       0.0090 -0.4848  0.0023 -0.0007 -0.0031
                                       0.0160  0.0020 -0.0134 -0.0006
            ( 39.32%)   0.6271* H 101 s( 99.96%)p 0.00(  0.04%)
                                      -0.9998 -0.0013 -0.0001 -0.0172 -0.0018
                                       0.0115
 97. (1.75785) BD ( 1) C  41 - C  42
            ( 44.52%)   0.6672* C  41 s( 37.96%)p 1.30( 49.31%)d 0.34( 12.73%)
                                       0.0000 -0.6133 -0.0553 -0.0197 -0.0027
                                       0.1738 -0.0779  0.0533  0.3260  0.0165
                                      -0.0382  0.5291 -0.2482  0.0670 -0.1555
                                       0.0408 -0.2973 -0.0180 -0.1130
            ( 55.48%)   0.7449* C  42 s( 33.58%)p 1.98( 66.37%)d 0.00(  0.05%)
                                       0.0000 -0.5794 -0.0030  0.0010  0.0000
                                      -0.1977 -0.0101  0.0001 -0.3551  0.0092
                                      -0.0019 -0.7059 -0.0035  0.0009 -0.0035
                                      -0.0108 -0.0139  0.0024 -0.0147
 98. (1.74502) BD ( 1) C  41 - C  46
            ( 43.76%)   0.6615* C  41 s( 36.17%)p 1.39( 50.23%)d 0.38( 13.60%)
                                      -0.0003  0.5978 -0.0609 -0.0258 -0.0025
                                       0.4202 -0.0918  0.0612 -0.3387  0.0307
                                      -0.0408  0.3585 -0.2513  0.0670 -0.1684
                                       0.0685 -0.3050 -0.0176 -0.0983
            ( 56.24%)   0.7499* C  46 s( 34.19%)p 1.92( 65.76%)d 0.00(  0.05%)
                                       0.0000  0.5847  0.0020 -0.0002  0.0001
                                      -0.4969  0.0013  0.0017  0.3954 -0.0085
                                       0.0026 -0.5041 -0.0105  0.0009 -0.0112
                                       0.0162 -0.0106  0.0022  0.0038
 99. (1.64949) BD ( 2) C  41 - C  46
            ( 52.75%)   0.7263* C  41 s(  0.04%)p99.99( 98.66%)d31.71(  1.30%)
                                      -0.0001 -0.0118  0.0141  0.0085  0.0011
                                       0.8228  0.0283 -0.0244  0.3815 -0.0045
                                       0.0080 -0.3956  0.0759 -0.0186  0.0462
                                      -0.0154  0.0984  0.0174  0.0260
            ( 47.25%)   0.6874* C  46 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                       0.0000  0.0021 -0.0037  0.0023  0.0000
                                       0.7900 -0.0074 -0.0041  0.4143 -0.0014
                                      -0.0003 -0.4514  0.0046 -0.0002 -0.0022
                                      -0.0093 -0.0084 -0.0097  0.0141
100. (1.97345) BD ( 1) C  42 - C  43
            ( 50.39%)   0.7099* C  42 s( 34.02%)p 1.94( 65.93%)d 0.00(  0.05%)
                                      -0.0001  0.5832  0.0088  0.0050  0.0002
                                       0.2753  0.0041  0.0005 -0.7415  0.0016
                                      -0.0070 -0.1828  0.0102 -0.0089 -0.0136
                                      -0.0013  0.0067 -0.0129 -0.0084
            ( 49.61%)   0.7043* C  43 s( 35.87%)p 1.79( 64.06%)d 0.00(  0.06%)
                                       0.0001  0.5989 -0.0004 -0.0039 -0.0003
                                      -0.3007 -0.0136  0.0026  0.7243  0.0129
                                      -0.0092  0.1581 -0.0100 -0.0053 -0.0146
                                      -0.0012  0.0090 -0.0152 -0.0090
101. (1.63619) BD ( 2) C  42 - C  43
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             ( 47.83%)   0.6916* C  42 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                       -0.0002  0.0002 -0.0028  0.0010  0.0001
                                        0.8064 -0.0066  0.0027  0.4056 -0.0017
                                       -0.0021 -0.4299  0.0017 -0.0012 -0.0069
                                       -0.0004  0.0089  0.0148 -0.0045
             ( 52.17%)   0.7223* C  43 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                        0.0000  0.0023  0.0003 -0.0005  0.0002
                                        0.7924 -0.0040  0.0130  0.4229 -0.0035
                                        0.0087 -0.4389  0.0043 -0.0083  0.0107
                                        0.0088 -0.0018 -0.0073 -0.0083
102. (1.96988) BD ( 1) C  42 - C  47
             ( 50.60%)   0.7114* C  42 s( 32.37%)p 2.09( 67.60%)d 0.00(  0.03%)
                                       -0.0001  0.5689 -0.0064 -0.0048 -0.0002
                                       -0.4840 -0.0068  0.0034  0.3985  0.0093
                                       -0.0061 -0.5316 -0.0132  0.0034 -0.0092
                                        0.0114 -0.0093 -0.0001  0.0027
             ( 49.40%)   0.7028* C  47 s( 26.33%)p 2.80( 73.61%)d 0.00(  0.06%)
                                        0.0002  0.5132 -0.0005  0.0010  0.0007
                                        0.4936 -0.0042 -0.0002 -0.4257  0.0009
                                       -0.0034  0.5579  0.0015  0.0008 -0.0116
                                        0.0157 -0.0134  0.0027  0.0026
103. (1.98096) BD ( 1) C  43 - C  44
             ( 50.07%)   0.7076* C  43 s( 35.86%)p 1.79( 64.08%)d 0.00(  0.05%)
                                        0.0000 -0.5987 -0.0137 -0.0045 -0.0002
                                       -0.4855 -0.0113 -0.0009  0.4007  0.0269
                                        0.0107 -0.4934  0.0064  0.0094  0.0091
                                       -0.0170  0.0093 -0.0036 -0.0064
             ( 49.93%)   0.7066* C  44 s( 35.97%)p 1.78( 63.96%)d 0.00(  0.07%)
                                        0.0000 -0.5997 -0.0065  0.0023  0.0001
                                        0.4876  0.0109 -0.0078 -0.3579  0.0108
                                        0.0123  0.5220  0.0287  0.0016  0.0159
                                       -0.0157  0.0125 -0.0004  0.0005
104. (1.97475) BD ( 1) C  43 - H  75
             ( 61.07%)   0.7815* C  43 s( 28.23%)p 2.54( 71.73%)d 0.00(  0.04%)
                                        0.0004 -0.5312  0.0110  0.0007 -0.0001
                                        0.2119 -0.0050 -0.0050  0.3668 -0.0028
                                       -0.0041  0.7331 -0.0148 -0.0114 -0.0034
                                       -0.0074 -0.0121  0.0022 -0.0121
             ( 38.93%)   0.6239* H  75 s( 99.94%)p 0.00(  0.06%)
                                       -0.9997  0.0021 -0.0014 -0.0069 -0.0098
                                       -0.0202
105. (1.98096) BD ( 1) C  44 - C  45
             ( 49.79%)   0.7056* C  44 s( 36.00%)p 1.78( 63.94%)d 0.00(  0.07%)
                                        0.0000  0.5999  0.0077 -0.0018 -0.0001
                                        0.2211  0.0194  0.0052  0.3173 -0.0121
                                       -0.0121  0.6989  0.0237 -0.0060  0.0028
                                        0.0082  0.0189 -0.0057  0.0138
             ( 50.21%)   0.7086* C  45 s( 36.09%)p 1.77( 63.86%)d 0.00(  0.05%)
                                        0.0000  0.6005  0.0145  0.0043  0.0000
                                       -0.1901  0.0105  0.0087 -0.3628 -0.0269
                                       -0.0111 -0.6854 -0.0074  0.0027  0.0029
                                        0.0122  0.0110 -0.0004  0.0153
106. (1.67441) BD ( 2) C  44 - C  45
             ( 48.91%)   0.6994* C  44 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                        0.0000  0.0020  0.0000  0.0013  0.0002
                                        0.7891 -0.0075  0.0086  0.4240 -0.0036
                                        0.0035 -0.4439  0.0042 -0.0045  0.0088
                                        0.0092 -0.0004 -0.0054 -0.0083
             ( 51.09%)   0.7148* C  45 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                                        0.0000  0.0006  0.0004  0.0008  0.0003
                                        0.7888 -0.0079  0.0174  0.4249 -0.0044
                                        0.0092 -0.4432  0.0044 -0.0094 -0.0024
                                       -0.0065 -0.0058 -0.0069  0.0101
107. (1.97752) BD ( 1) C  44 - H  74
             ( 60.87%)   0.7802* C  44 s( 27.98%)p 2.57( 71.99%)d 0.00(  0.03%)
                                        0.0004 -0.5288  0.0120 -0.0037 -0.0003
                                       -0.2992  0.0092 -0.0021  0.7682 -0.0213
                                        0.0037  0.1992 -0.0055  0.0010  0.0075
                                        0.0069 -0.0052  0.0098  0.0099
             ( 39.13%)   0.6255* H  74 s( 99.95%)p 0.00(  0.05%)
                                       -0.9997 -0.0015 -0.0005  0.0081 -0.0208
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                                    -0.0056
108. (1.97278) BD ( 1) C  45 - C  46
             ( 49.52%)   0.7037* C  45 s( 35.81%)p 1.79( 64.13%)d 0.00(  0.06%)
                                     0.0001  0.5984 -0.0015 -0.0044 -0.0001
                                    -0.2685  0.0021  0.0054  0.7226  0.0119
                                    -0.0097  0.2157  0.0166 -0.0008 -0.0144
                                    -0.0012  0.0096 -0.0151 -0.0088
             ( 50.48%)   0.7105* C  46 s( 33.92%)p 1.95( 66.03%)d 0.00(  0.05%)
                                    -0.0001  0.5823  0.0105  0.0032  0.0001
                                     0.2821 -0.0061  0.0072 -0.7397  0.0039
                                    -0.0067 -0.1828 -0.0064  0.0029 -0.0123
                                    -0.0015  0.0091 -0.0133 -0.0076
109. (1.97534) BD ( 1) C  45 - H  73
             ( 60.77%)   0.7795* C  45 s( 28.08%)p 2.56( 71.89%)d 0.00(  0.04%)
                                    -0.0004  0.5298 -0.0108 -0.0003  0.0001
                                     0.5182 -0.0097 -0.0075 -0.4053  0.0025
                                     0.0044  0.5345 -0.0133 -0.0097 -0.0095
                                     0.0131 -0.0096  0.0024  0.0022
             ( 39.23%)   0.6264* H  73 s( 99.95%)p 0.00(  0.05%)
                                     0.9997  0.0022  0.0013 -0.0141  0.0109
                                    -0.0148
110. (1.96959) BD ( 1) C  46 - C  49
             ( 50.02%)   0.7072* C  46 s( 31.86%)p 2.14( 68.11%)d 0.00(  0.03%)
                                    -0.0001  0.5644 -0.0068 -0.0036 -0.0001
                                     0.2210  0.0078 -0.0009  0.3522  0.0054
                                    -0.0021  0.7127  0.0147 -0.0044  0.0028
                                     0.0079  0.0115 -0.0023  0.0105
             ( 49.98%)   0.7070* C  49 s( 26.68%)p 2.75( 73.27%)d 0.00(  0.06%)
                                     0.0001  0.5165  0.0013 -0.0016 -0.0001
                                    -0.2369 -0.0022  0.0021 -0.3571  0.0024
                                     0.0001 -0.7410  0.0012  0.0030  0.0047
                                     0.0095  0.0147 -0.0019  0.0149
111. (1.96910) BD ( 1) C  47 - C  48
             ( 50.59%)   0.7113* C  47 s( 25.46%)p 2.93( 74.50%)d 0.00(  0.04%)
                                    -0.0001  0.5044 -0.0108  0.0010 -0.0002
                                     0.4860 -0.0006  0.0000  0.4814  0.0109
                                     0.0039 -0.5263 -0.0032 -0.0033  0.0111
                                    -0.0120 -0.0111  0.0025  0.0007
             ( 49.41%)   0.7029* C  48 s( 29.04%)p 2.44( 70.91%)d 0.00(  0.04%)
                                     0.0004  0.5385 -0.0197 -0.0031  0.0001
                                    -0.4637 -0.0097  0.0063 -0.4668 -0.0057
                                     0.0107  0.5252  0.0065 -0.0089  0.0111
                                    -0.0124 -0.0129 -0.0003  0.0017
112. (1.97975) BD ( 1) C  47 - C  57
             ( 51.04%)   0.7144* C  47 s( 26.39%)p 2.79( 73.57%)d 0.00(  0.04%)
                                    -0.0001  0.5136 -0.0115  0.0020 -0.0004
                                    -0.4881 -0.0114 -0.0033 -0.5405  0.0046
                                    -0.0014 -0.4528  0.0053 -0.0020  0.0124
                                     0.0097  0.0115 -0.0027 -0.0006
             ( 48.96%)   0.6997* C  57 s( 29.01%)p 2.45( 70.94%)d 0.00(  0.05%)
                                     0.0002  0.5382 -0.0202 -0.0029  0.0000
                                     0.5103  0.0053 -0.0120  0.4975  0.0106
                                    -0.0068  0.4483  0.0050 -0.0073  0.0139
                                     0.0123  0.0117  0.0007 -0.0021
113. (1.95741) BD ( 1) C  47 - H  80
             ( 63.35%)   0.7959* C  47 s( 21.87%)p 3.57( 78.08%)d 0.00(  0.05%)
                                     0.0001 -0.4673 -0.0194  0.0039  0.0000
                                     0.5302 -0.0013 -0.0029 -0.5421  0.0107
                                     0.0021 -0.4533  0.0094  0.0071  0.0137
                                     0.0119 -0.0123  0.0010  0.0018
             ( 36.65%)   0.6054* H  80 s( 99.95%)p 0.00(  0.05%)
                                    -0.9997  0.0068 -0.0009 -0.0164  0.0118
                                     0.0100
114. (1.98559) BD ( 1) C  48 - H 126
             ( 60.94%)   0.7807* C  48 s( 23.30%)p 3.29( 76.66%)d 0.00(  0.04%)
                                     0.0001 -0.4827 -0.0059 -0.0020 -0.0001
                                     0.5128 -0.0049 -0.0032 -0.4359  0.0020
                                    -0.0064  0.5599 -0.0050  0.0055  0.0111
                                    -0.0139  0.0110 -0.0012 -0.0022
             ( 39.06%)   0.6250* H 126 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0016 -0.0002 -0.0143  0.0089
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                                    -0.0115
115. (1.98706) BD ( 1) C  48 - H 127
             ( 60.67%)   0.7789* C  48 s( 24.01%)p 3.16( 75.94%)d 0.00(  0.05%)
                                     0.0000  0.4899  0.0038  0.0015 -0.0001
                                     0.4783 -0.0029  0.0042  0.5823 -0.0008
                                     0.0058  0.4376 -0.0025 -0.0072  0.0126
                                     0.0115  0.0138 -0.0024 -0.0038
             ( 39.33%)   0.6272* H 127 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0016  0.0000 -0.0094 -0.0139
                                    -0.0122
116. (1.98982) BD ( 1) C  48 - H 128
             ( 60.43%)   0.7774* C  48 s( 23.65%)p 3.23( 76.31%)d 0.00(  0.05%)
                                    -0.0001  0.4862  0.0077  0.0000  0.0000
                                     0.5408  0.0011  0.0065 -0.5023  0.0043
                                     0.0042 -0.4672  0.0000 -0.0061 -0.0135
                                    -0.0111  0.0119  0.0021 -0.0015
             ( 39.57%)   0.6290* H 128 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0023  0.0002 -0.0126  0.0141
                                     0.0110
117. (1.97532) BD ( 1) C  49 - C  50
             ( 50.69%)   0.7120* C  49 s( 25.91%)p 2.86( 74.05%)d 0.00(  0.04%)
                                    -0.0001  0.5089 -0.0121  0.0007  0.0000
                                     0.8477  0.0045  0.0039  0.1466  0.0136
                                     0.0017  0.0129  0.0021  0.0017  0.0045
                                    -0.0004  0.0006  0.0162 -0.0095
             ( 49.31%)   0.7022* C  50 s( 29.25%)p 2.42( 70.71%)d 0.00(  0.05%)
                                     0.0003  0.5405 -0.0189 -0.0035  0.0001
                                    -0.8273 -0.0121  0.0145 -0.1479  0.0011
                                     0.0049 -0.0197  0.0025  0.0008  0.0068
                                     0.0005  0.0002  0.0170 -0.0107
118. (1.97545) BD ( 1) C  49 - C  58
             ( 51.06%)   0.7146* C  49 s( 26.33%)p 2.80( 73.64%)d 0.00(  0.04%)
                                    -0.0001  0.5130 -0.0114  0.0010  0.0001
                                    -0.2341 -0.0099  0.0001 -0.4865  0.0074
                                    -0.0017  0.6668  0.0074  0.0067  0.0055
                                    -0.0063 -0.0149 -0.0048  0.0069
             ( 48.94%)   0.6996* C  58 s( 29.00%)p 2.45( 70.96%)d 0.00(  0.05%)
                                     0.0003  0.5383 -0.0139  0.0007 -0.0004
                                     0.2375  0.0047 -0.0061  0.4655  0.0082
                                    -0.0040 -0.6605 -0.0035  0.0083  0.0059
                                    -0.0087 -0.0158 -0.0042  0.0090
119. (1.96417) BD ( 1) C  49 - H  79
             ( 61.47%)   0.7840* C  49 s( 21.13%)p 3.73( 78.82%)d 0.00(  0.05%)
                                    -0.0002  0.4592  0.0199 -0.0003  0.0001
                                    -0.4117  0.0059  0.0063  0.7829 -0.0133
                                    -0.0022  0.0741  0.0010  0.0059 -0.0162
                                    -0.0014  0.0028 -0.0113 -0.0113
             ( 38.53%)   0.6207* H  79 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0054  0.0001  0.0108 -0.0183
                                    -0.0007
120. (1.98629) BD ( 1) C  50 - H 129
             ( 60.74%)   0.7793* C  50 s( 23.28%)p 3.29( 76.68%)d 0.00(  0.04%)
                                    -0.0001  0.4824  0.0052  0.0022  0.0001
                                     0.2253  0.0008  0.0084  0.4023 -0.0020
                                     0.0031  0.7444 -0.0062  0.0012  0.0041
                                     0.0082  0.0138 -0.0034  0.0125
             ( 39.26%)   0.6266* H 129 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0015  0.0002 -0.0034 -0.0096
                                    -0.0183
121. (1.98839) BD ( 1) C  50 - H 130
             ( 60.58%)   0.7783* C  50 s( 23.73%)p 3.21( 76.22%)d 0.00(  0.05%)
                                     0.0000  0.4871  0.0069  0.0001 -0.0001
                                     0.4523  0.0047  0.0092 -0.7450  0.0039
                                     0.0006 -0.0499 -0.0012 -0.0002 -0.0169
                                    -0.0011  0.0018 -0.0089 -0.0092
             ( 39.42%)   0.6279* H 130 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0023  0.0002 -0.0099  0.0191
                                     0.0016
122. (1.98804) BD ( 1) C  50 - H 131
             ( 60.81%)   0.7798* C  50 s( 23.75%)p 3.21( 76.21%)d 0.00(  0.05%)
                                    -0.0001  0.4873  0.0045  0.0015 -0.0001
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                                     0.2428  0.0013  0.0091  0.5105 -0.0030
                                     0.0027 -0.6651  0.0042  0.0005  0.0055
                                    -0.0083 -0.0156 -0.0064  0.0086
             ( 39.19%)   0.6260* H 131 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0013  0.0001 -0.0050 -0.0122
                                     0.0157
123. (1.97541) BD ( 1) C  51 - C  52
             ( 50.70%)   0.7120* C  51 s( 25.89%)p 2.86( 74.08%)d 0.00(  0.04%)
                                    -0.0001  0.5087 -0.0118  0.0006  0.0000
                                     0.5288  0.0133  0.0036  0.6263  0.0001
                                     0.0006  0.2621 -0.0059  0.0016  0.0145
                                     0.0063  0.0076 -0.0037 -0.0071
             ( 49.30%)   0.7022* C  52 s( 29.26%)p 2.42( 70.70%)d 0.00(  0.04%)
                                     0.0003  0.5406 -0.0187 -0.0032  0.0001
                                    -0.5262 -0.0040  0.0109 -0.6035 -0.0111
                                     0.0100 -0.2560 -0.0041  0.0035  0.0166
                                     0.0066  0.0077 -0.0022 -0.0079
124. (1.97561) BD ( 1) C  51 - C  59
             ( 51.02%)   0.7143* C  51 s( 26.38%)p 2.79( 73.58%)d 0.00(  0.04%)
                                    -0.0001  0.5135 -0.0118  0.0012  0.0000
                                    -0.2026  0.0029  0.0020 -0.5190 -0.0130
                                    -0.0038  0.6521 -0.0027  0.0054  0.0049
                                    -0.0062 -0.0148 -0.0042  0.0073
             ( 48.98%)   0.6999* C  59 s( 28.97%)p 2.45( 70.99%)d 0.00(  0.05%)
                                     0.0003  0.5379 -0.0183 -0.0028  0.0001
                                     0.1861  0.0069 -0.0027  0.5215  0.0055
                                    -0.0103 -0.6348 -0.0075  0.0083  0.0053
                                    -0.0064 -0.0175 -0.0064  0.0071
125. (1.96408) BD ( 1) C  51 - H  81
             ( 61.45%)   0.7839* C  51 s( 21.11%)p 3.73( 78.83%)d 0.00(  0.05%)
                                    -0.0002  0.4591  0.0199 -0.0002  0.0001
                                     0.4307 -0.0066  0.0046 -0.4807  0.0063
                                     0.0017 -0.6095  0.0112  0.0073 -0.0105
                                    -0.0134  0.0148 -0.0009  0.0047
             ( 38.55%)   0.6209* H  81 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0053  0.0003 -0.0094  0.0114
                                     0.0157
126. (1.98624) BD ( 1) C  52 - H 114
             ( 60.73%)   0.7793* C  52 s( 23.27%)p 3.30( 76.69%)d 0.00(  0.04%)
                                    -0.0001  0.4824  0.0049  0.0019  0.0002
                                     0.7336 -0.0036  0.0070 -0.3472  0.0045
                                     0.0056  0.3286 -0.0026  0.0021 -0.0125
                                     0.0111 -0.0057  0.0102 -0.0053
             ( 39.27%)   0.6266* H 114 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0015  0.0002 -0.0170  0.0101
                                    -0.0074
127. (1.98831) BD ( 1) C  52 - H 115
             ( 60.84%)   0.7800* C  52 s( 23.73%)p 3.21( 76.23%)d 0.00(  0.05%)
                                    -0.0001  0.4871  0.0049  0.0015 -0.0001
                                     0.2238 -0.0001  0.0067  0.5221 -0.0009
                                     0.0061 -0.6629  0.0057  0.0021  0.0040
                                    -0.0078 -0.0171 -0.0052  0.0073
             ( 39.16%)   0.6258* H 115 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0012  0.0001 -0.0049 -0.0122
                                     0.0160
128. (1.98844) BD ( 1) C  52 - H 116
             ( 60.58%)   0.7783* C  52 s( 23.74%)p 3.21( 76.21%)d 0.00(  0.05%)
                                     0.0000  0.4872  0.0066  0.0001 -0.0001
                                    -0.3660  0.0049  0.0048  0.4916  0.0039
                                     0.0069  0.6215 -0.0014  0.0034 -0.0098
                                    -0.0107  0.0141 -0.0030  0.0062
             ( 39.42%)   0.6279* H 116 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0023  0.0002  0.0102 -0.0118
                                    -0.0149
129. (1.96921) BD ( 1) C  53 - C  54
             ( 50.53%)   0.7109* C  53 s( 25.43%)p 2.93( 74.53%)d 0.00(  0.04%)
                                    -0.0001  0.5041 -0.0116  0.0012 -0.0002
                                     0.4120  0.0070  0.0017  0.6126 -0.0008
                                     0.0013 -0.4473 -0.0101 -0.0040  0.0131
                                    -0.0073 -0.0118 -0.0058 -0.0031
             ( 49.47%)   0.7033* C  54 s( 29.16%)p 2.43( 70.79%)d 0.00(  0.04%)
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                                     0.0004  0.5397 -0.0197 -0.0026  0.0001
                                    -0.3913 -0.0065  0.0080 -0.5986 -0.0106
                                     0.0085  0.4428  0.0038 -0.0097  0.0122
                                    -0.0092 -0.0136 -0.0052 -0.0016
130. (1.97956) BD ( 1) C  53 - C  60
             ( 51.23%)   0.7158* C  53 s( 26.68%)p 2.75( 73.28%)d 0.00(  0.04%)
                                    -0.0001  0.5164 -0.0111  0.0030 -0.0003
                                    -0.8357  0.0002 -0.0037  0.0020 -0.0130
                                    -0.0010 -0.1850 -0.0039 -0.0027 -0.0012
                                     0.0066 -0.0012  0.0163 -0.0085
             ( 48.77%)   0.6984* C  60 s( 28.89%)p 2.46( 71.06%)d 0.00(  0.05%)
                                     0.0002  0.5372 -0.0153 -0.0008 -0.0003
                                     0.8143  0.0103 -0.0109  0.0251  0.0000
                                    -0.0036  0.2162 -0.0030 -0.0031  0.0017
                                     0.0094  0.0008  0.0178 -0.0091
131. (1.95860) BD ( 1) C  53 - H  82
             ( 62.84%)   0.7927* C  53 s( 21.59%)p 3.63( 78.36%)d 0.00(  0.05%)
                                     0.0002 -0.4642 -0.0196  0.0045  0.0001
                                    -0.3373  0.0117  0.0022  0.7826 -0.0088
                                    -0.0066  0.2390 -0.0015  0.0035  0.0136
                                     0.0042 -0.0084  0.0116  0.0090
             ( 37.16%)   0.6096* H  82 s( 99.95%)p 0.00(  0.05%)
                                    -0.9997  0.0062 -0.0008  0.0052 -0.0204
                                    -0.0064
132. (1.98561) BD ( 1) C  54 - H 117
             ( 60.91%)   0.7804* C  54 s( 23.30%)p 3.29( 76.66%)d 0.00(  0.04%)
                                     0.0002 -0.4826 -0.0057 -0.0020 -0.0001
                                     0.1218 -0.0024 -0.0046  0.1206 -0.0013
                                    -0.0045  0.8585 -0.0068  0.0062  0.0001
                                    -0.0048 -0.0054 -0.0005 -0.0198
             ( 39.09%)   0.6252* H 117 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0016 -0.0002 -0.0044 -0.0051
                                    -0.0192
133. (1.98955) BD ( 1) C  54 - H 118
             ( 60.47%)   0.7777* C  54 s( 23.65%)p 3.23( 76.30%)d 0.00(  0.05%)
                                     0.0000  0.4863  0.0077 -0.0003  0.0000
                                    -0.3074  0.0038  0.0041  0.7912  0.0001
                                     0.0079  0.2058 -0.0023 -0.0041 -0.0116
                                    -0.0016  0.0086 -0.0127 -0.0087
             ( 39.53%)   0.6287* H 118 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0024  0.0002  0.0090 -0.0189
                                    -0.0062
134. (1.98730) BD ( 1) C  54 - H 119
             ( 60.54%)   0.7781* C  54 s( 23.89%)p 3.18( 76.06%)d 0.00(  0.05%)
                                     0.0000  0.4887  0.0041  0.0013 -0.0001
                                     0.8584 -0.0030  0.0039 -0.0069 -0.0003
                                     0.0068  0.1538 -0.0025 -0.0064 -0.0010
                                     0.0071  0.0021  0.0185 -0.0098
             ( 39.46%)   0.6282* H 119 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0015  0.0000 -0.0201  0.0025
                                    -0.0038
135. (1.98449) BD ( 1) C  55 - H 108
             ( 60.68%)   0.7790* C  55 s( 23.12%)p 3.32( 76.84%)d 0.00(  0.04%)
                                    -0.0002  0.4808  0.0082  0.0040  0.0002
                                    -0.6195  0.0084 -0.0010  0.5849 -0.0036
                                     0.0137  0.2050 -0.0088  0.0044 -0.0172
                                    -0.0052  0.0061  0.0019 -0.0080
             ( 39.32%)   0.6271* H 108 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0014  0.0004  0.0156 -0.0129
                                    -0.0053
136. (1.98741) BD ( 1) C  55 - H 109
             ( 60.54%)   0.7781* C  55 s( 23.70%)p 3.22( 76.26%)d 0.00(  0.04%)
                                     0.0000  0.4867  0.0104  0.0020 -0.0001
                                     0.6609  0.0017  0.0052  0.1029  0.0056
                                     0.0091  0.5612 -0.0090  0.0058  0.0022
                                     0.0172  0.0035  0.0106  0.0021
             ( 39.46%)   0.6281* H 109 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0022  0.0005 -0.0161 -0.0015
                                    -0.0143
137. (1.98644) BD ( 1) C  55 - H 110
             ( 62.17%)   0.7885* C  55 s( 24.50%)p 3.08( 75.45%)d 0.00(  0.05%)
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                                    -0.0001  0.4949 -0.0072 -0.0057  0.0004
                                     0.2873  0.0032 -0.0034  0.1782  0.0096
                                     0.0006 -0.7999 -0.0022  0.0116  0.0025
                                    -0.0118 -0.0074  0.0015  0.0174
             ( 37.83%)   0.6151* H 110 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0013  0.0005 -0.0067 -0.0041
                                     0.0190
138. (1.98436) BD ( 1) C  56 - H 102
             ( 60.79%)   0.7796* C  56 s( 23.09%)p 3.33( 76.87%)d 0.00(  0.04%)
                                     0.0001 -0.4804 -0.0089  0.0041 -0.0003
                                     0.1249 -0.0045 -0.0059  0.4190 -0.0112
                                     0.0062  0.7598 -0.0050  0.0113 -0.0016
                                    -0.0052 -0.0150  0.0034 -0.0124
             ( 39.21%)   0.6262* H 102 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0012 -0.0004 -0.0046 -0.0103
                                    -0.0177
139. (1.98632) BD ( 1) C  56 - H 103
             ( 62.31%)   0.7894* C  56 s( 24.65%)p 3.05( 75.30%)d 0.00(  0.05%)
                                    -0.0001  0.4964 -0.0083  0.0062  0.0004
                                     0.1525  0.0073 -0.0016  0.8364  0.0016
                                    -0.0132 -0.1727 -0.0074  0.0005  0.0066
                                    -0.0012 -0.0073 -0.0176 -0.0098
             ( 37.69%)   0.6139* H 103 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0011  0.0006 -0.0026 -0.0199
                                     0.0040
140. (1.98716) BD ( 1) C  56 - H 104
             ( 60.37%)   0.7770* C  56 s( 23.63%)p 3.23( 76.33%)d 0.00(  0.04%)
                                     0.0000  0.4860  0.0113 -0.0023 -0.0002
                                     0.7103  0.0046  0.0105 -0.3397  0.0091
                                    -0.0063  0.3781 -0.0071 -0.0016 -0.0117
                                     0.0129 -0.0048  0.0092 -0.0039
             ( 39.63%)   0.6295* H 104 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0021  0.0004 -0.0171  0.0087
                                    -0.0098
141. (1.98474) BD ( 1) C  57 - H 123
             ( 61.50%)   0.7842* C  57 s( 23.50%)p 3.25( 76.46%)d 0.00(  0.04%)
                                     0.0001 -0.4847 -0.0041 -0.0020 -0.0001
                                     0.5723  0.0021  0.0032 -0.4761  0.0065
                                     0.0046  0.4584 -0.0106  0.0079  0.0142
                                    -0.0113  0.0100 -0.0025  0.0011
             ( 38.50%)   0.6205* H 123 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0012 -0.0004 -0.0127  0.0134
                                    -0.0083
142. (1.98872) BD ( 1) C  57 - H 124
             ( 59.98%)   0.7745* C  57 s( 23.56%)p 3.24( 76.39%)d 0.00(  0.04%)
                                     0.0000 -0.4854 -0.0081 -0.0006 -0.0002
                                    -0.4578  0.0030  0.0070  0.4864  0.0027
                                     0.0058  0.5635  0.0010  0.0083  0.0117
                                     0.0125 -0.0117  0.0013 -0.0034
             ( 40.02%)   0.6326* H 124 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0023 -0.0003  0.0119 -0.0110
                                    -0.0138
143. (1.98684) BD ( 1) C  57 - H 125
             ( 61.30%)   0.7829* C  57 s( 23.93%)p 3.18( 76.03%)d 0.00(  0.05%)
                                     0.0001 -0.4891 -0.0053 -0.0007  0.0002
                                     0.4490  0.0059  0.0027  0.5368 -0.0079
                                     0.0076 -0.5200  0.0042  0.0040 -0.0100
                                     0.0131  0.0132  0.0020 -0.0001
             ( 38.70%)   0.6221* H 125 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0011 -0.0002 -0.0108 -0.0112
                                     0.0135
144. (1.98532) BD ( 1) C  58 - H 132
             ( 60.64%)   0.7787* C  58 s( 23.09%)p 3.33( 76.87%)d 0.00(  0.04%)
                                    -0.0001  0.4804  0.0080  0.0036  0.0002
                                     0.2234 -0.0081  0.0016  0.3950 -0.0048
                                    -0.0023  0.7500 -0.0068  0.0126  0.0032
                                     0.0085  0.0141 -0.0025  0.0120
             ( 39.36%)   0.6274* H 132 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0014  0.0004 -0.0059 -0.0111
                                    -0.0167
145. (1.98713) BD ( 1) C  58 - H 133
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            ( 61.82%)   0.7863* C  58 s( 24.40%)p 3.10( 75.55%)d 0.00(  0.05%)
                                        0.0001 -0.4939  0.0070  0.0052 -0.0004
                                        0.8601  0.0056 -0.0119  0.1241  0.0047
                                       -0.0003 -0.0054 -0.0077 -0.0028 -0.0057
                                        0.0005 -0.0003 -0.0187  0.0115
            ( 38.18%)   0.6179* H 133 s( 99.96%)p 0.00(  0.04%)
                                       -0.9998 -0.0014 -0.0005 -0.0201 -0.0021
                                       -0.0004
146. (1.98795) BD ( 1) C  58 - H 134
            ( 60.31%)   0.7766* C  58 s( 23.52%)p 3.25( 76.43%)d 0.00(  0.04%)
                                        0.0000 -0.4849 -0.0112 -0.0019  0.0002
                                       -0.3910  0.0078 -0.0021  0.7816 -0.0017
                                        0.0107  0.0156 -0.0035 -0.0073  0.0146
                                       -0.0010 -0.0014  0.0108  0.0106
            ( 39.69%)   0.6300* H 134 s( 99.95%)p 0.00(  0.05%)
                                       -0.9998 -0.0022 -0.0004  0.0102 -0.0189
                                       -0.0016
147. (1.98540) BD ( 1) C  59 - H 111
            ( 60.59%)   0.7784* C  59 s( 23.12%)p 3.32( 76.83%)d 0.00(  0.04%)
                                       -0.0001  0.4808  0.0062  0.0028  0.0002
                                        0.7326 -0.0062 -0.0007 -0.3229 -0.0010
                                       -0.0064  0.3567 -0.0033  0.0094 -0.0117
                                        0.0122 -0.0040  0.0104 -0.0051
            ( 39.41%)   0.6278* H 111 s( 99.96%)p 0.00(  0.04%)
                                        0.9998  0.0015  0.0003 -0.0185  0.0068
                                       -0.0076
148. (1.98797) BD ( 1) C  59 - H 112
            ( 60.42%)   0.7773* C  59 s( 23.63%)p 3.23( 76.33%)d 0.00(  0.04%)
                                        0.0000  0.4861  0.0067  0.0010  0.0000
                                       -0.4396 -0.0039 -0.0004  0.4197 -0.0069
                                       -0.0036  0.6274  0.0004  0.0087 -0.0091
                                       -0.0121  0.0129  0.0015  0.0056
            ( 39.58%)   0.6291* H 112 s( 99.95%)p 0.00(  0.05%)
                                        0.9998  0.0022  0.0004  0.0106 -0.0117
                                       -0.0148
149. (1.98638) BD ( 1) C  59 - H 113
            ( 61.73%)   0.7857* C  59 s( 24.28%)p 3.12( 75.68%)d 0.00(  0.05%)
                                        0.0001 -0.4927 -0.0030  0.0004  0.0002
                                        0.4846  0.0001 -0.0024  0.6685 -0.0025
                                        0.0050  0.2739 -0.0040 -0.0062 -0.0150
                                       -0.0067 -0.0093  0.0044  0.0090
            ( 38.27%)   0.6186* H 113 s( 99.96%)p 0.00(  0.04%)
                                       -0.9998 -0.0012  0.0001 -0.0108 -0.0140
                                       -0.0087
150. (1.98440) BD ( 1) C  60 - H 120
            ( 61.42%)   0.7837* C  60 s( 23.28%)p 3.29( 76.67%)d 0.00(  0.04%)
                                        0.0001 -0.4824 -0.0097 -0.0039  0.0000
                                        0.0866  0.0017  0.0098  0.1992  0.0066
                                       -0.0015  0.8480 -0.0147  0.0107  0.0006
                                       -0.0031 -0.0079  0.0023 -0.0189
            ( 38.58%)   0.6211* H 120 s( 99.96%)p 0.00(  0.04%)
                                       -0.9998 -0.0010 -0.0004  0.0003 -0.0066
                                       -0.0194
151. (1.98692) BD ( 1) C  60 - H 121
            ( 61.76%)   0.7859* C  60 s( 24.34%)p 3.11( 75.61%)d 0.00(  0.05%)
                                       -0.0001  0.4933 -0.0075 -0.0046  0.0002
                                       -0.4301 -0.0099  0.0043 -0.5960 -0.0072
                                        0.0087  0.4643 -0.0061 -0.0081  0.0134
                                       -0.0108 -0.0142 -0.0045 -0.0019
            ( 38.24%)   0.6184* H 121 s( 99.96%)p 0.00(  0.04%)
                                        0.9998  0.0011  0.0005  0.0084  0.0155
                                       -0.0093
152. (1.98826) BD ( 1) C  60 - H 122
            ( 59.83%)   0.7735* C  60 s( 23.50%)p 3.25( 76.46%)d 0.00(  0.04%)
                                        0.0000  0.4846  0.0110  0.0022  0.0001
                                       -0.3784 -0.0047 -0.0115  0.7770 -0.0058
                                        0.0074  0.1321  0.0001 -0.0044 -0.0143
                                       -0.0025  0.0044 -0.0116 -0.0083
            ( 40.17%)   0.6338* H 122 s( 99.95%)p 0.00(  0.05%)
                                        0.9998  0.0022  0.0004  0.0079 -0.0195
                                       -0.0032
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153. (1.98496) BD ( 1) C  61 - H  96
             ( 60.62%)   0.7786* C  61 s( 23.12%)p 3.32( 76.84%)d 0.00(  0.04%)
                                      -0.0001  0.4807  0.0079  0.0038  0.0002
                                      -0.0046  0.0065  0.0014  0.2164 -0.0009
                                       0.0106  0.8493 -0.0096  0.0083 -0.0013
                                      -0.0001  0.0080 -0.0012  0.0189
             ( 39.38%)   0.6276* H  96 s( 99.96%)p 0.00(  0.04%)
                                       0.9998  0.0014  0.0004  0.0009 -0.0037
                                      -0.0205
154. (1.98679) BD ( 1) C  61 - H  97
             ( 61.97%)   0.7872* C  61 s( 24.44%)p 3.09( 75.51%)d 0.00(  0.05%)
                                      -0.0001  0.4943 -0.0071 -0.0055  0.0004
                                       0.8263  0.0065 -0.0111 -0.0357  0.0087
                                       0.0030 -0.2660  0.0016  0.0048 -0.0014
                                      -0.0112  0.0003  0.0177 -0.0078
             ( 38.03%)   0.6167* H  97 s( 99.96%)p 0.00(  0.04%)
                                       0.9998  0.0014  0.0005 -0.0195  0.0012
                                       0.0061
155. (1.98764) BD ( 1) C  61 - H  98
             ( 60.49%)   0.7777* C  61 s( 23.60%)p 3.24( 76.36%)d 0.00(  0.04%)
                                       0.0000  0.4857  0.0110  0.0019 -0.0002
                                      -0.4043  0.0101 -0.0012  0.6376  0.0009
                                       0.0127 -0.4397  0.0012 -0.0006 -0.0130
                                       0.0080 -0.0128 -0.0059 -0.0014
             ( 39.51%)   0.6286* H  98 s( 99.95%)p 0.00(  0.05%)
                                       0.9998  0.0021  0.0003  0.0107 -0.0148
                                       0.0114
156. (1.98463) BD ( 1) C  62 - H  87
             ( 60.62%)   0.7786* C  62 s( 22.95%)p 3.36( 77.01%)d 0.00(  0.04%)
                                      -0.0001  0.4790  0.0048  0.0031  0.0001
                                       0.4665  0.0025  0.0026 -0.7245  0.0094
                                      -0.0016 -0.1651 -0.0002 -0.0088 -0.0160
                                      -0.0020  0.0059 -0.0077 -0.0091
             ( 39.38%)   0.6276* H  87 s( 99.96%)p 0.00(  0.04%)
                                       0.9998  0.0010  0.0004 -0.0104  0.0174
                                       0.0020
157. (1.98761) BD ( 1) C  62 - H  88
             ( 60.03%)   0.7748* C  62 s( 23.44%)p 3.26( 76.52%)d 0.00(  0.05%)
                                       0.0000  0.4841  0.0073  0.0009  0.0001
                                      -0.6110  0.0038  0.0039  0.0685  0.0033
                                      -0.0011 -0.6221 -0.0039 -0.0118 -0.0025
                                       0.0190 -0.0006  0.0079  0.0045
             ( 39.97%)   0.6322* H  88 s( 99.96%)p 0.00(  0.04%)
                                       0.9998  0.0022  0.0003  0.0154 -0.0015
                                       0.0145
158. (1.98595) BD ( 1) C  62 - H  89
             ( 63.18%)   0.7948* C  62 s( 25.12%)p 2.98( 74.84%)d 0.00(  0.05%)
                                      -0.0001  0.5011  0.0065 -0.0008 -0.0002
                                       0.5279  0.0010  0.0013  0.6832 -0.0088
                                       0.0011 -0.0533  0.0011 -0.0090  0.0174
                                       0.0007 -0.0019 -0.0040 -0.0120
             ( 36.82%)   0.6068* H  89 s( 99.95%)p 0.00(  0.05%)
                                       0.9997  0.0022  0.0000 -0.0130 -0.0184
                                      -0.0042
159. (1.99867) CR ( 1) C   1           s(100.00%)p 0.00(  0.00%)
                                       1.0000  0.0003  0.0000  0.0000  0.0000
                                       0.0000  0.0000  0.0000 -0.0001  0.0000
                                       0.0000 -0.0002  0.0000  0.0000  0.0000
                                       0.0000  0.0000  0.0000  0.0000
160. (1.99981) CR ( 1) O   2           s(100.00%)p 0.00(  0.00%)
                                       1.0000  0.0003  0.0000  0.0000  0.0000
                                       0.0000  0.0000  0.0000  0.0001  0.0000
                                       0.0000 -0.0002  0.0000  0.0000  0.0000
                                       0.0000  0.0000  0.0000  0.0000
161. (1.99898) CR ( 1) C   3           s(100.00%)p 0.00(  0.00%)
                                       1.0000  0.0002  0.0000  0.0000  0.0000
                                       0.0001  0.0000  0.0000  0.0002  0.0000
                                       0.0000 -0.0001  0.0000  0.0000  0.0000
                                       0.0000  0.0000  0.0000  0.0000
162. (1.99875) CR ( 1) C   4           s(100.00%)p 0.00(  0.00%)
                                       1.0000  0.0004  0.0000  0.0000  0.0000
```

```
                                      0.0001  0.0000  0.0000  0.0001  0.0000
                                      0.0000 -0.0001  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  163. (1.99898) CR ( 1) C   5      s(100.00%)
                                      1.0000  0.0002  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000  0.0000
                                      0.0000  0.0001  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  164. (1.99910) CR ( 1) C   6      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0002  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0001  0.0000
                                      0.0000  0.0003  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  165. (1.99920) CR ( 1) C   7      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0002  0.0000  0.0000  0.0000
                                     -0.0002  0.0000  0.0000  0.0002  0.0000
                                      0.0000  0.0002  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  166. (1.99910) CR ( 1) C   8      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0002  0.0000  0.0000  0.0000
                                     -0.0003  0.0000  0.0000  0.0002  0.0000
                                      0.0000 -0.0001  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  167. (1.99944) CR ( 1) N   9      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0002  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000  0.0000
                                      0.0000  0.0001  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  168. (1.99868) CR ( 1) C  10      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0004  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0002  0.0000
                                      0.0000 -0.0003  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  169. (1.99943) CR ( 1) N  11      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0002  0.0000  0.0000  0.0000
                                      0.0001  0.0000  0.0000  0.0000  0.0000
                                      0.0000  0.0001  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  170. (1.99903) CR ( 1) C  12      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0003  0.0000  0.0000  0.0000
                                      0.0002  0.0000  0.0000 -0.0001  0.0000
                                      0.0000 -0.0001  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  171. (1.99902) CR ( 1) C  13      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0003  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0002  0.0000
                                      0.0000  0.0000  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  172. (1.99760) CR ( 1) B  14      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0021  0.0000  0.0000  0.0000
                                     -0.0016  0.0000  0.0000  0.0003  0.0000
                                      0.0000 -0.0040  0.0000  0.0000  0.0000
                                      0.0001  0.0000  0.0000  0.0001
  173. (1.99700) CR ( 1) B  15      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0011  0.0000  0.0000  0.0000
                                     -0.0012  0.0000  0.0000 -0.0002  0.0000
                                      0.0000 -0.0007  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  174. (1.99876) CR ( 1) C  16      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0003  0.0000  0.0000  0.0000
                                     -0.0002  0.0000  0.0000 -0.0003  0.0000
                                      0.0000  0.0000  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  175. (1.99942) CR ( 1) N  17      s(100.00%)
                                      1.0000  0.0002  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0001  0.0000
                                      0.0000  0.0000  0.0000  0.0000  0.0000
                                      0.0000  0.0000  0.0000  0.0000
  176. (1.99904) CR ( 1) C  18      s(100.00%)p 0.00(  0.00%)
                                      1.0000  0.0003  0.0000  0.0000  0.0000
                                     -0.0002  0.0000  0.0000  0.0000  0.0000
```

```
                                     0.0000 -0.0001  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
177. (1.99904) CR ( 1) C  19          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0003  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000 -0.0001  0.0000
                                     0.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
178. (1.99942) CR ( 1) N  20          s(100.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
179. (1.99873) CR ( 1) C  21          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0004  0.0000  0.0000  0.0000
                                    -0.0001  0.0000  0.0000 -0.0001  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
180. (1.99897) CR ( 1) C  22          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                    -0.0002  0.0000  0.0000 -0.0001  0.0000
                                     0.0000 -0.0001  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
181. (1.99910) CR ( 1) C  23          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                    -0.0001  0.0000  0.0000  0.0000  0.0000
                                     0.0000 -0.0004  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
182. (1.99920) CR ( 1) C  24          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                    -0.0002  0.0000  0.0000  0.0002  0.0000
                                     0.0000 -0.0003  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
183. (1.99909) CR ( 1) C  25          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0001  0.0000  0.0000  0.0000
                                    -0.0002  0.0000  0.0000  0.0003  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
184. (1.99898) CR ( 1) C  26          s(100.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0001  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
185. (1.99936) CR ( 1) C  27          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0001  0.0000  0.0000  0.0000
                                     0.0001  0.0000  0.0000 -0.0002  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
186. (1.99941) CR ( 1) C  28          s(100.00%)p 0.00(  0.00%)
                                     1.0000 -0.0001  0.0000  0.0000  0.0000
                                    -0.0002  0.0000  0.0000 -0.0003  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
187. (1.99937) CR ( 1) C  29          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0001  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
188. (1.99942) CR ( 1) C  30          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0000  0.0000  0.0000  0.0000
                                    -0.0003  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
189. (1.99874) CR ( 1) C  31          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0004  0.0000  0.0000  0.0000
                                    -0.0001  0.0000  0.0000 -0.0001  0.0000
                                     0.0000  0.0001  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
190. (1.99898) CR ( 1) C  32          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0001  0.0000  0.0000  0.0000
```

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                                    0.0000  0.0000  0.0000  0.0000
191. (1.99910) CR ( 1) C  33          s(100.00%)p 0.00(  0.00%)
                                    1.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0001  0.0000  0.0000  0.0001  0.0000
                                    0.0000  0.0004  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
192. (1.99920) CR ( 1) C  34          s(100.00%)p 0.00(  0.00%)
                                    1.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0003  0.0000  0.0000 -0.0001  0.0000
                                    0.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
193. (1.99910) CR ( 1) C  35          s(100.00%)p 0.00(  0.00%)
                                    1.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0003  0.0000  0.0000 -0.0002  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
194. (1.99898) CR ( 1) C  36          s(100.00%)
                                    1.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0001  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
195. (1.99937) CR ( 1) C  37          s(100.00%)p 0.00(  0.00%)
                                    1.0000  0.0001  0.0000  0.0000  0.0000
                                   -0.0002  0.0000  0.0000  0.0001  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
196. (1.99942) CR ( 1) C  38          s(100.00%)p 0.00(  0.00%)
                                    1.0000  0.0000  0.0000  0.0000  0.0000
                                   -0.0002  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0003  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
197. (1.99936) CR ( 1) C  39          s(100.00%)p 0.00(  0.00%)
                                    1.0000  0.0001  0.0000  0.0000  0.0000
                                   -0.0001  0.0000  0.0000 -0.0001  0.0000
                                    0.0000 -0.0002  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
198. (1.99942) CR ( 1) C  40          s(100.00%)p 0.00(  0.00%)
                                    1.0000 -0.0001  0.0000  0.0000  0.0000
                                   -0.0001  0.0000  0.0000 -0.0004  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
199. (1.99874) CR ( 1) C  41          s(100.00%)p 0.00(  0.00%)d 0.00(  0.00%)
                                    1.0000  0.0003 -0.0001  0.0000  0.0000
                                    0.0001 -0.0001  0.0001  0.0002  0.0000
                                    0.0000 -0.0003 -0.0003  0.0001 -0.0002
                                    0.0001 -0.0004  0.0000 -0.0001
200. (1.99899) CR ( 1) C  42          s(100.00%)p 0.00(  0.00%)
                                    1.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0001  0.0000  0.0000  0.0000  0.0000
                                    0.0000 -0.0002  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
201. (1.99911) CR ( 1) C  43          s(100.00%)p 0.00(  0.00%)
                                    1.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000 -0.0002  0.0000
                                    0.0000 -0.0003  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
202. (1.99920) CR ( 1) C  44          s(100.00%)p 0.00(  0.00%)
                                    1.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0002  0.0000  0.0000 -0.0003  0.0000
                                    0.0000 -0.0001  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
203. (1.99909) CR ( 1) C  45          s(100.00%)p 0.00(  0.00%)
                                    1.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0003  0.0000  0.0000 -0.0002  0.0000
                                    0.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
204. (1.99898) CR ( 1) C  46          s(100.00%)
                                    1.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000 -0.0001  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000
```

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205. (1.99935) CR ( 1) C  47          s(100.00%)p 0.00(  0.00%)
                                        1.0000  0.0001  0.0000  0.0000  0.0000
                                       -0.0001  0.0000  0.0000  0.0002  0.0000
                                        0.0000 -0.0001  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
206. (1.99941) CR ( 1) C  48          s(100.00%)p 0.00(  0.00%)
                                        1.0000 -0.0001  0.0000  0.0000  0.0000
                                        0.0002  0.0000  0.0000  0.0002  0.0000
                                        0.0000 -0.0003  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
207. (1.99936) CR ( 1) C  49          s(100.00%)p 0.00(  0.00%)
                                        1.0000  0.0001  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0002  0.0000
                                        0.0000  0.0002  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
208. (1.99942) CR ( 1) C  50          s(100.00%)p 0.00(  0.00%)
                                        1.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0003  0.0000  0.0000  0.0001  0.0000
                                        0.0000  0.0001  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
209. (1.99937) CR ( 1) C  51          s(100.00%)p 0.00(  0.00%)
                                        1.0000  0.0001  0.0000  0.0000  0.0000
                                        0.0002  0.0000  0.0000 -0.0001  0.0000
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
210. (1.99942) CR ( 1) C  52          s(100.00%)p 0.00(  0.00%)
                                        1.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0003  0.0000  0.0000  0.0002  0.0000
                                        0.0000  0.0001  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
211. (1.99935) CR ( 1) C  53          s(100.00%)p 0.00(  0.00%)
                                        1.0000  0.0001  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000 -0.0001  0.0000
                                        0.0000 -0.0002  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
212. (1.99941) CR ( 1) C  54          s(100.00%)p 0.00(  0.00%)
                                        1.0000 -0.0001  0.0000  0.0000  0.0000
                                        0.0002  0.0000  0.0000  0.0003  0.0000
                                        0.0000 -0.0003  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
213. (1.99941) CR ( 1) C  55          s(100.00%)p 0.00(  0.00%)
                                        1.0000 -0.0001  0.0000  0.0000  0.0000
                                        0.0001  0.0000  0.0000  0.0004  0.0000
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
214. (1.99942) CR ( 1) C  56          s(100.00%)p 0.00(  0.00%)
                                        1.0000 -0.0001  0.0000  0.0000  0.0000
                                        0.0002  0.0000  0.0000  0.0000  0.0000
                                        0.0000 -0.0003  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
215. (1.99943) CR ( 1) C  57          s(100.00%)p 0.00(  0.00%)
                                        1.0000  0.0000  0.0000  0.0000  0.0000
                                       -0.0002  0.0000  0.0000 -0.0001  0.0000
                                        0.0000 -0.0001  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
216. (1.99942) CR ( 1) C  58          s(100.00%)p 0.00(  0.00%)
                                        1.0000 -0.0001  0.0000  0.0000  0.0000
                                       -0.0001  0.0000  0.0000 -0.0001  0.0000
                                        0.0000  0.0003  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
217. (1.99941) CR ( 1) C  59          s(100.00%)p 0.00(  0.00%)
                                        1.0000 -0.0001  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000 -0.0002  0.0000
                                        0.0000  0.0002  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
218. (1.99943) CR ( 1) C  60          s(100.00%)p 0.00(  0.00%)
                                        1.0000  0.0000  0.0000  0.0000  0.0000
                                       -0.0003  0.0000  0.0000 -0.0001  0.0000
                                        0.0000 -0.0001  0.0000  0.0000  0.0000
                                        0.0000  0.0000  0.0000  0.0000
219. (1.99942) CR ( 1) C  61          s(100.00%)p 0.00(  0.00%)
```

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                                     1.0000 -0.0001  0.0000  0.0000  0.0000
                                     0.0002  0.0000  0.0000  0.0003  0.0000
                                     0.0000  0.0001  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
220. (1.99942) CR ( 1) C  62       s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0002  0.0000  0.0000  0.0000  0.0000
                                     0.0000 -0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000
221. (1.96474) LP ( 1) O   2       s( 59.74%)p 0.67( 40.24%)d 0.00(  0.02%)
                                    -0.0003  0.7729  0.0095 -0.0003 -0.0002
                                    -0.0745  0.0003 -0.0013  0.1686  0.0008
                                     0.0015 -0.6070 -0.0059 -0.0055  0.0006
                                    -0.0035  0.0063 -0.0004 -0.0117
222. (1.74913) LP ( 2) O   2       s(  0.28%)p99.99( 99.65%)d 0.22(  0.06%)
                                     0.0001  0.0533 -0.0014 -0.0009 -0.0001
                                    -0.9537 -0.0129  0.0018 -0.2737 -0.0047
                                     0.0008  0.1088  0.0000 -0.0012  0.0046
                                    -0.0220 -0.0068 -0.0068  0.0056
223. (0.58308) LP*( 1) B  14       s(  0.06%)p99.99( 99.79%)d 2.25(  0.14%)
                                     0.0000  0.0252  0.0004 -0.0006 -0.0017
                                    -0.4664  0.0010  0.0107  0.8415  0.0036
                                    -0.0234  0.2674  0.0014 -0.0105 -0.0246
                                     0.0004 -0.0201  0.0155 -0.0136
224. (0.74839) LP ( 1) B  15       s(  0.01%)p 1.00( 99.92%)d 0.00(  0.07%)
                                     0.0000  0.0097  0.0020 -0.0007 -0.0006
                                    -0.3649 -0.0035  0.0097  0.8632  0.0133
                                    -0.0213  0.3465  0.0082 -0.0072  0.0042
                                     0.0111 -0.0176 -0.0138 -0.0102
225. (1.53944) LP ( 1) N  20       s(  0.01%)p 1.00( 99.98%)d 0.00(  0.01%)
                                     0.0000  0.0081 -0.0020  0.0011  0.0000
                                     0.2547  0.0046  0.0023 -0.7226 -0.0075
                                    -0.0074 -0.6423 -0.0096 -0.0065  0.0066
                                     0.0037  0.0016 -0.0004  0.0058
226. (0.01705) RY*( 1) C   1       s( 24.47%)p 3.06( 74.95%)d 0.02(  0.58%)
                                     0.0000 -0.0522  0.4916 -0.0158 -0.0065
                                     0.0060  0.1757  0.0274 -0.0208 -0.2056
                                    -0.0149  0.0707  0.8172  0.0468 -0.0296
                                     0.0622  0.0202  0.0020  0.0255
227. (0.00521) RY*( 2) C   1       s(  0.18%)p28.27(  4.96%)d99.99( 94.87%)
                                     0.0000  0.0004  0.0244  0.0339  0.0030
                                    -0.0123 -0.0740  0.0539  0.0465  0.0357
                                    -0.1744  0.0168  0.0036 -0.0829  0.2744
                                    -0.2261  0.7617  0.1212  0.4769
228. (0.00290) RY*( 3) C   1       s( 14.31%)p 0.58(  8.25%)d 5.41( 77.44%)
                                     0.0000 -0.0044 -0.2414  0.2911 -0.0048
                                     0.0121  0.1941 -0.0036  0.0043  0.0039
                                    -0.0738 -0.0156  0.1809  0.0790  0.2034
                                    -0.7947 -0.2581 -0.1849 -0.0269
229. (0.00155) RY*( 4) C   1       s( 40.18%)p 0.45( 17.95%)d 1.04( 41.87%)
                                     0.0000 -0.0039  0.5562 -0.3042 -0.0026
                                     0.0139  0.1285 -0.0175 -0.0110  0.2132
                                     0.0587  0.0451 -0.3028 -0.1406 -0.1299
                                    -0.2382 -0.2678 -0.2596  0.4538
230. (0.00086) RY*( 5) C   1       s(  3.61%)p25.78( 92.98%)d 0.95(  3.41%)
                                     0.0000  0.0013  0.1663  0.0915  0.0057
                                     0.0120 -0.6197 -0.5299  0.0009 -0.4213
                                    -0.2774  0.0060 -0.0558  0.0853 -0.0121
                                    -0.0935 -0.1150 -0.0895  0.0630
231. (0.00055) RY*( 6) C   1       s(  0.63%)p99.99( 99.28%)d 0.15(  0.09%)
                                     0.0000 -0.0008 -0.0046  0.0787 -0.0061
                                    -0.0037 -0.4514 -0.2028  0.0057  0.7697
                                     0.2333  0.0003  0.3017  0.0999  0.0168
                                    -0.0052 -0.0115 -0.0224  0.0015
232. (0.00041) RY*( 7) C   1       s( 86.66%)p 0.13( 11.33%)d 0.02(  2.01%)
                                     0.0000  0.0081  0.4245  0.8282 -0.0185
                                     0.0094  0.0147  0.1286 -0.0054  0.0140
                                     0.1769  0.0308 -0.2433 -0.0697 -0.0257
                                     0.0685  0.0634  0.0261 -0.1003
233. (0.00029) RY*( 8) C   1       s(  1.71%)p55.64( 95.10%)d 1.87(  3.19%)
                                     0.0000  0.0131  0.1033  0.0778 -0.0140
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                                    -0.0017  0.4479 -0.4123 -0.0008  0.2714
                                    -0.4617 -0.0001 -0.1239  0.5274 -0.0265
                                     0.1305  0.0795  0.0672 -0.0579
234. (0.00015) RY*( 9) C   1        s(  1.70%)p57.16( 97.19%)d 0.65(  1.10%)
                                     0.0000  0.0272  0.1082 -0.0675  0.0001
                                     0.0053 -0.3178  0.6403  0.0011 -0.0284
                                    -0.1467 -0.0026 -0.0620  0.6594 -0.0434
                                    -0.0583 -0.0528 -0.0428  0.0337
235. (0.00010) RY*(10) C   1        s( 24.73%)p 0.27(  6.72%)d 2.77( 68.55%)
                                     0.0000  0.0175  0.3773 -0.3233 -0.0065
                                    -0.0014 -0.0414 -0.0682 -0.0036  0.0038
                                     0.1748  0.0152 -0.1700  0.0338  0.3822
                                    -0.2920  0.1464  0.2900 -0.5904
236. (0.00008) RY*(11) C   1        s(  0.96%)p94.46( 90.88%)d 8.48(  8.16%)
237. (0.00002) RY*(12) C   1        s(  2.00%)p 0.26(  0.52%)d48.71( 97.48%)
238. (0.00002) RY*(13) C   1        s(  2.25%)p 0.25(  0.57%)d43.20( 97.18%)
239. (0.00000) RY*(14) C   1        s( 96.26%)p 0.00(  0.05%)d 0.04(  3.69%)
240. (0.00533) RY*( 1) O   2        s(  1.14%)p83.64( 95.57%)d 2.88(  3.29%)
                                     0.0000  0.0001  0.1065 -0.0087  0.0017
                                    -0.0083  0.9109 -0.0039 -0.0023  0.3387
                                     0.0036  0.0039 -0.1030 -0.0210  0.0205
                                    -0.1566 -0.0663 -0.0528  0.0278
241. (0.00361) RY*( 2) O   2        s(  0.47%)p99.99( 97.97%)d 3.36(  1.56%)
                                     0.0000 -0.0006  0.0682 -0.0008  0.0001
                                    -0.0044 -0.3160  0.0025  0.0153  0.9007
                                     0.0007  0.0037  0.2615 -0.0082 -0.0312
                                     0.0207 -0.1009 -0.0214 -0.0599
242. (0.00179) RY*( 3) O   2        s( 86.63%)p 0.15( 13.34%)d 0.00(  0.02%)
                                     0.0000 -0.0035  0.9306  0.0162  0.0089
                                     0.0030 -0.1331 -0.0385 -0.0025 -0.0351
                                     0.0424  0.0135 -0.2843 -0.1738  0.0101
                                    -0.0078  0.0021  0.0082  0.0005
243. (0.00041) RY*( 4) O   2        s(  7.88%)p11.53( 90.77%)d 0.17(  1.35%)
                                     0.0000  0.0262  0.2692 -0.0733 -0.0155
                                     0.0060  0.1504 -0.0264 -0.0065 -0.2372
                                    -0.0017  0.0291  0.9037 -0.1032 -0.0267
                                    -0.0536 -0.0023  0.0085 -0.0992
244. (0.00004) RY*( 5) O   2        s( 45.37%)p 1.02( 46.36%)d 0.18(  8.27%)
245. (0.00001) RY*( 6) O   2        s(  0.28%)p99.99( 99.70%)d 0.06(  0.02%)
246. (0.00001) RY*( 7) O   2        s( 13.96%)p 6.17( 86.04%)d 0.00(  0.00%)
247. (0.00001) RY*( 8) O   2        s(  0.13%)p12.37(  1.60%)d99.99( 98.27%)
248. (0.00001) RY*( 9) O   2        s( 40.12%)p 1.49( 59.87%)d 0.00(  0.01%)
249. (0.00001) RY*(10) O   2        s(  0.16%)p 2.34(  0.37%)d99.99( 99.47%)
250. (0.00001) RY*(11) O   2        s(  0.97%)p 3.57(  3.48%)d98.15( 95.55%)
251. (0.00001) RY*(12) O   2        s(  2.53%)p 1.64(  4.14%)d36.86( 93.33%)
252. (0.00001) RY*(13) O   2        s(  0.56%)p 1.69(  0.95%)d99.99( 98.49%)
253. (0.00000) RY*(14) O   2        s( 99.85%)p 0.00(  0.09%)d 0.00(  0.06%)
254. (0.00513) RY*( 1) C   3        s(  0.68%)p99.99( 92.50%)d 9.97(  6.82%)
                                     0.0000  0.0025  0.0370  0.0739 -0.0026
                                     0.0077 -0.3570 -0.0255  0.0000  0.0374
                                     0.0147  0.0239 -0.8910  0.0273  0.1092
                                    -0.0406  0.1147 -0.0717  0.1905
255. (0.00305) RY*( 2) C   3        s(  5.18%)p16.55( 85.65%)d 1.77(  9.18%)
                                     0.0000 -0.0020  0.2225 -0.0475  0.0018
                                     0.0043  0.7445  0.0251  0.0017 -0.4416
                                    -0.0027  0.0025 -0.3245 -0.0352  0.0830
                                     0.2420 -0.0900  0.1243  0.0525
256. (0.00254) RY*( 3) C   3        s(  4.47%)p19.28( 86.25%)d 2.07(  9.28%)
                                     0.0000  0.0029  0.2072  0.0422  0.0037
                                     0.0027 -0.4401 -0.0638 -0.0024 -0.7880
                                    -0.0692 -0.0006  0.1683  0.1033  0.0044
                                    -0.1546 -0.2107  0.0440  0.1502
257. (0.00148) RY*( 4) C   3        s( 85.65%)p 0.16( 13.53%)d 0.01(  0.83%)
                                     0.0000 -0.0031  0.9216 -0.0846 -0.0046
                                     0.0025 -0.0678  0.1899  0.0036  0.2852
                                    -0.0778 -0.0121  0.0607  0.0580 -0.0289
                                    -0.0566  0.0418  0.0432 -0.0248
258. (0.00077) RY*( 5) C   3        s(  5.76%)p 6.64( 38.23%)d 9.73( 56.01%)
                                     0.0000 -0.0059  0.1653  0.1733  0.0135
                                     0.0024  0.0948 -0.3749 -0.0140 -0.0323
                                     0.4420 -0.0020  0.0293  0.1879 -0.2220
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                                    0.0798 -0.0109 -0.7101 -0.0054
259. (0.00043) RY*( 6) C   3      s(  5.03%)p17.58( 88.41%)d 1.31(  6.57%)
                                    0.0000  0.0007 -0.1040  0.1978  0.0181
                                   -0.0036  0.0401  0.3718 -0.0017 -0.0088
                                    0.0060  0.0082  0.0421  0.8615  0.1731
                                    0.1210  0.1427  0.0246 -0.0075
260. (0.00040) RY*( 7) C   3      s(  0.75%)p41.94( 31.45%)d90.44( 67.81%)
                                    0.0000 -0.0053  0.0759 -0.0403  0.0092
                                    0.0084  0.0488 -0.4635 -0.0153 -0.1046
                                    0.2698 -0.0035  0.0340  0.1098  0.0984
                                   -0.2652  0.6416  0.3937 -0.1773
261. (0.00036) RY*( 8) C   3      s( 79.12%)p 0.14( 11.18%)d 0.12(  9.69%)
                                    0.0000  0.0018  0.0871  0.8851 -0.0149
                                    0.0016  0.0664 -0.2351  0.0015  0.1346
                                   -0.1459 -0.0069  0.0514 -0.1002  0.1590
                                   -0.0197 -0.1706  0.1979  0.0547
262. (0.00024) RY*( 9) C   3      s(  1.85%)p 9.26( 17.09%)d43.92( 81.07%)
                                    0.0000  0.0032  0.0572  0.1232 -0.0013
                                   -0.0165 -0.2518  0.0787 -0.0083 -0.1663
                                   -0.1060 -0.0001  0.0660 -0.2402  0.1409
                                    0.7163  0.3851 -0.1179 -0.3398
263. (0.00014) RY*(10) C   3      s(  3.74%)p 3.76( 14.07%)d21.98( 82.19%)
                                    0.0000  0.0007 -0.0293  0.1909 -0.0088
                                    0.0005  0.0479  0.1846 -0.0045 -0.1413
                                   -0.1983 -0.0111 -0.2106  0.0230 -0.5309
                                   -0.2931  0.0073 -0.0329 -0.6730
264. (0.00012) RY*(11) C   3      s(  2.97%)p 9.93( 29.46%)d22.78( 67.57%)
                                    0.0000  0.0050 -0.0238  0.1703 -0.0090
                                    0.0130  0.1769  0.3579 -0.0101 -0.1419
                                   -0.1949  0.0008  0.1089 -0.2549  0.1666
                                   -0.3987  0.4937 -0.4136  0.2725
265. (0.00008) RY*(12) C   3      s(  3.13%)p29.14( 91.29%)d 1.78(  5.58%)
266. (0.00004) RY*(13) C   3      s(  2.02%)p 0.48(  0.96%)d48.13( 97.02%)
267. (0.00000) RY*(14) C   3      s( 99.69%)p 0.00(  0.09%)d 0.00(  0.22%)
268. (0.00649) RY*( 1) C   4      s(  5.75%)p15.12( 87.01%)d 1.26(  7.24%)
                                    0.0000  0.0068  0.2354  0.0457  0.0019
                                   -0.0096  0.5147  0.0031  0.0157 -0.6198
                                   -0.0517  0.0096 -0.4667 -0.0113 -0.0899
                                   -0.2079  0.1180 -0.0338 -0.0773
269. (0.00335) RY*( 2) C   4      s(  0.09%)p99.99( 96.05%)d41.98(  3.86%)
                                    0.0000 -0.0014  0.0302  0.0012 -0.0020
                                    0.0039  0.5981 -0.1252 -0.0001  0.7139
                                    0.0672 -0.0028 -0.2682  0.0296 -0.0385
                                    0.0652  0.0485 -0.1594 -0.0716
270. (0.00249) RY*( 3) C   4      s(  1.53%)p56.28( 85.95%)d 8.20( 12.53%)
                                    0.0000  0.0030  0.1232 -0.0085  0.0026
                                    0.0088 -0.5300  0.0430 -0.0013  0.1560
                                   -0.0175  0.0050 -0.7428  0.0101 -0.1323
                                    0.0787 -0.1686  0.0734 -0.2603
271. (0.00113) RY*( 4) C   4      s( 54.55%)p 0.62( 33.97%)d 0.21( 11.49%)
                                    0.0000 -0.0057  0.7315 -0.1013  0.0001
                                    0.0007  0.0447  0.1463  0.0047  0.0828
                                   -0.2608  0.0070  0.2493 -0.4234 -0.0257
                                    0.2217 -0.0852  0.1188 -0.2090
272. (0.00080) RY*( 5) C   4      s(  2.02%)p 3.62(  7.30%)d44.90( 90.68%)
                                    0.0000 -0.0011  0.0314  0.1386 -0.0022
                                    0.0035 -0.0133  0.0440  0.0105  0.0361
                                   -0.1466 -0.0007 -0.0067 -0.2190 -0.2965
                                   -0.3085 -0.6046 -0.4319  0.4141
273. (0.00069) RY*( 6) C   4      s( 44.25%)p 0.43( 18.92%)d 0.83( 36.83%)
                                    0.0000  0.0026 -0.2797  0.6035  0.0004
                                    0.0002  0.0735 -0.2547 -0.0017 -0.0640
                                    0.0512  0.0127  0.1388 -0.3046 -0.2052
                                    0.0435 -0.1748  0.1229 -0.5279
274. (0.00058) RY*( 7) C   4      s( 51.46%)p 0.59( 30.36%)d 0.35( 18.18%)
                                    0.0000 -0.0022  0.1491  0.7016  0.0064
                                   -0.0084 -0.0458  0.5002  0.0089  0.1495
                                   -0.1133 -0.0008 -0.0600  0.1116  0.2581
                                   -0.1383  0.2280  0.0745  0.1963
275. (0.00041) RY*( 8) C   4      s( 23.13%)p 2.53( 58.49%)d 0.79( 18.38%)
                                    0.0000  0.0054  0.4007  0.2659 -0.0060
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                                    -0.0058 -0.2090 -0.7158 -0.0046 -0.0237
                                     0.1640 -0.0069 -0.0123  0.0322  0.2289
                                     0.0063  0.1777 -0.2438  0.2009
276. (0.00038) RY*( 9) C   4        s(  2.43%)p26.53( 64.55%)d13.57( 33.02%)
                                     0.0000  0.0003  0.1519 -0.0341  0.0096
                                     0.0118  0.0649  0.0880  0.0055  0.0347
                                     0.7696 -0.0059 -0.0243 -0.1980  0.1179
                                    -0.2223 -0.2560  0.4247  0.1447
277. (0.00033) RY*(10) C   4        s( 10.15%)p 6.58( 66.72%)d 2.28( 23.13%)
                                     0.0000  0.0023  0.3049  0.0923  0.0010
                                     0.0077  0.0462  0.0664 -0.0038 -0.0397
                                     0.1598  0.0046  0.2205  0.7648 -0.1885
                                     0.0298 -0.3350 -0.0796 -0.2763
278. (0.00012) RY*(11) C   4        s(  2.38%)p 3.64(  8.64%)d37.46( 88.98%)
                                     0.0000 -0.0056  0.1158 -0.1005  0.0148
                                    -0.0115 -0.1709 -0.0162  0.0132  0.1793
                                     0.0335  0.0118  0.1508 -0.0228 -0.4475
                                    -0.6812  0.4372 -0.0030 -0.1853
279. (0.00010) RY*(12) C   4        s(  0.04%)p99.99( 39.77%)d99.99( 60.19%)
                                     0.0000  0.0013 -0.0053 -0.0109  0.0169
                                    -0.0017 -0.0856  0.3448 -0.0016 -0.0997
                                     0.4694  0.0007  0.0299 -0.2007  0.0038
                                     0.2152  0.2044 -0.6831 -0.2171
280. (0.00005) RY*(13) C   4        s(  2.45%)p 0.96(  2.35%)d38.90( 95.21%)
281. (0.00000) RY*(14) C   4        s( 99.82%)p 0.00(  0.06%)d 0.00(  0.12%)
282. (0.00510) RY*( 1) C   5        s(  0.71%)p99.99( 92.35%)d 9.75(  6.94%)
                                     0.0000  0.0012  0.0092  0.0838 -0.0015
                                    -0.0180  0.6166 -0.0335  0.0080 -0.2812
                                     0.0087 -0.0148  0.6800 -0.0064 -0.1200
                                     0.0290 -0.0858  0.0821 -0.2001
283. (0.00298) RY*( 2) C   5        s(  1.73%)p51.82( 89.66%)d 4.98(  8.61%)
                                     0.0000  0.0013  0.1314 -0.0047  0.0047
                                    -0.0032 -0.0355 -0.0109 -0.0028 -0.8832
                                    -0.0727 -0.0033 -0.3309  0.0220  0.1558
                                     0.1860 -0.0060  0.1644  0.0132
284. (0.00284) RY*( 3) C   5        s(  6.26%)p13.76( 86.18%)d 1.21(  7.56%)
                                     0.0000 -0.0019  0.2501 -0.0073  0.0046
                                     0.0014  0.7076  0.0641  0.0013  0.2088
                                     0.0753 -0.0051 -0.5546  0.0063 -0.0513
                                     0.1158 -0.2002 -0.1026  0.0945
285. (0.00148) RY*( 4) C   5        s( 90.77%)p 0.07(  6.54%)d 0.03(  2.69%)
                                     0.0000 -0.0038  0.9516 -0.0468 -0.0044
                                     0.0145 -0.1588  0.0403 -0.0031  0.0681
                                    -0.0163  0.0000  0.1824 -0.0137  0.0114
                                    -0.1102  0.1090  0.0520  0.0023
286. (0.00067) RY*( 5) C   5        s(  0.56%)p10.43(  5.79%)d99.99( 93.65%)
                                     0.0000 -0.0019  0.0176  0.0723  0.0047
                                     0.0108  0.0553 -0.0212  0.0121  0.0751
                                     0.1935 -0.0064 -0.0348  0.0992  0.1657
                                     0.5009  0.6409 -0.2619 -0.4229
287. (0.00049) RY*( 6) C   5        s(  9.08%)p 7.61( 69.14%)d 2.40( 21.78%)
                                     0.0000  0.0070  0.0236  0.3003  0.0000
                                    -0.0072 -0.0488  0.1314  0.0092  0.1029
                                    -0.3121  0.0109  0.0680 -0.7476  0.2285
                                     0.3738 -0.1570 -0.0077  0.0330
288. (0.00041) RY*( 7) C   5        s( 51.28%)p 0.74( 38.19%)d 0.21( 10.53%)
                                     0.0000 -0.0004  0.0720  0.7125  0.0063
                                     0.0010 -0.0864 -0.5170 -0.0113 -0.0648
                                     0.2944 -0.0055 -0.1098 -0.0637 -0.1516
                                    -0.1956 -0.1051 -0.1515 -0.1000
289. (0.00028) RY*( 8) C   5        s( 32.91%)p 1.79( 58.94%)d 0.25(  8.15%)
                                     0.0000 -0.0005  0.0118  0.5733 -0.0160
                                     0.0047 -0.0556  0.4845  0.0000  0.0755
                                    -0.1739  0.0055  0.0649  0.5580  0.1180
                                     0.1667 -0.1228  0.0980  0.1229
290. (0.00021) RY*( 9) C   5        s(  2.29%)p 4.57( 10.48%)d38.05( 87.23%)
                                     0.0000  0.0001 -0.0628  0.1378  0.0001
                                     0.0080  0.1854 -0.1474  0.0094  0.1718
                                    -0.0526 -0.0055 -0.1141 -0.0564  0.3541
                                    -0.2666  0.3391  0.7457 -0.0692
291. (0.00013) RY*(10) C   5        s(  0.13%)p99.99( 14.66%)d99.99( 85.20%)
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                                     0.0000 -0.0032 -0.0143  0.0316 -0.0102
                                     0.0022  0.1517 -0.2859  0.0011 -0.0458
                                    -0.0538  0.0148  0.1790  0.0683  0.3241
                                     0.0186  0.2922 -0.2708  0.7668
292. (0.00011) RY*(11) C   5        s(  3.81%)p 9.75( 37.17%)d15.48( 59.02%)
                                     0.0000  0.0004 -0.0594  0.1860  0.0030
                                     0.0089  0.1205  0.4862 -0.0104 -0.1791
                                    -0.1112 -0.0044 -0.1040 -0.2556 -0.2106
                                    -0.5275  0.4444 -0.2642  0.0164
293. (0.00007) RY*(12) C   5        s(  0.11%)p99.99( 85.97%)d99.99( 13.92%)
294. (0.00004) RY*(13) C   5        s(  1.19%)p 4.08(  4.87%)d78.76( 93.94%)
295. (0.00000) RY*(14) C   5        s( 99.18%)p 0.00(  0.19%)d 0.01(  0.62%)
296. (0.00409) RY*( 1) C   6        s(  1.65%)p54.27( 89.36%)d 5.47(  9.00%)
                                     0.0000  0.0055  0.1269 -0.0176  0.0032
                                    -0.0071 -0.2344  0.1050 -0.0037 -0.1589
                                    -0.0688 -0.0236 -0.8916 -0.0461  0.1638
                                     0.0570  0.0491 -0.0536  0.2337
297. (0.00143) RY*( 2) C   6        s(  0.31%)p99.99( 98.56%)d 3.70(  1.13%)
                                     0.0000  0.0072  0.0532  0.0101  0.0085
                                    -0.0219  0.8256  0.0151  0.0189 -0.5275
                                    -0.0844  0.0028 -0.1180 -0.0611 -0.0388
                                     0.0606 -0.0589  0.0487 -0.0168
298. (0.00131) RY*( 3) C   6        s(  0.03%)p99.99( 91.64%)d99.99(  8.33%)
                                     0.0000  0.0004  0.0160 -0.0062 -0.0002
                                     0.0115  0.4240 -0.1737  0.0091  0.7529
                                    -0.2559 -0.0038 -0.2474  0.1129  0.0113
                                    -0.1521 -0.1402  0.1700  0.1069
299. (0.00060) RY*( 4) C   6        s( 93.76%)p 0.04(  3.69%)d 0.03(  2.55%)
                                     0.0000 -0.0009  0.9589 -0.1347 -0.0046
                                     0.0164 -0.0228  0.0998 -0.0064  0.0446
                                    -0.0170  0.0170  0.1244  0.0898  0.0297
                                     0.0681 -0.1043 -0.0056 -0.0954
300. (0.00048) RY*( 5) C   6        s(  0.08%)p99.99(  8.98%)d99.99( 90.94%)
                                     0.0000 -0.0005  0.0278  0.0047 -0.0050
                                     0.0051 -0.1300 -0.0875  0.0077 -0.1884
                                    -0.1425 -0.0016  0.0668  0.0699  0.2907
                                    -0.1957  0.1894  0.8664 -0.0043
301. (0.00015) RY*( 6) C   6        s(  1.33%)p18.94( 25.28%)d54.99( 73.39%)
                                     0.0000 -0.0045  0.1123  0.0179 -0.0197
                                    -0.0163  0.0962 -0.1892  0.0141 -0.0842
                                     0.2177  0.0084  0.0209  0.3903  0.0125
                                    -0.5980  0.4866 -0.2684  0.2594
302. (0.00009) RY*( 7) C   6        s(  4.03%)p17.00( 68.52%)d 6.81( 27.45%)
303. (0.00005) RY*( 8) C   6        s(  7.37%)p 3.05( 22.46%)d 9.53( 70.17%)
304. (0.00006) RY*( 9) C   6        s(  1.37%)p51.39( 70.30%)d20.72( 28.34%)
305. (0.00006) RY*(10) C   6        s( 47.29%)p 0.95( 45.01%)d 0.16(  7.70%)
306. (0.00002) RY*(11) C   6        s( 12.04%)p 2.73( 32.84%)d 4.58( 55.12%)
307. (0.00001) RY*(12) C   6        s( 32.23%)p 0.87( 28.09%)d 1.23( 39.68%)
308. (0.00002) RY*(13) C   6        s(  1.09%)p14.05( 15.36%)d76.40( 83.54%)
309. (0.00000) RY*(14) C   6        s( 97.45%)p 0.00(  0.04%)d 0.03(  2.50%)
310. (0.00412) RY*( 1) C   7        s(  0.99%)p91.53( 90.94%)d 8.12(  8.07%)
                                     0.0000  0.0005  0.0892  0.0441  0.0064
                                     0.0191  0.5604 -0.0366 -0.0187 -0.5668
                                     0.0268 -0.0168 -0.5194  0.0357 -0.0660
                                    -0.2258  0.1207 -0.0461 -0.0929
311. (0.00185) RY*( 2) C   7        s(  0.07%)p99.99( 99.93%)d 0.07(  0.00%)
                                     0.0000 -0.0003  0.0256  0.0016  0.0010
                                    -0.0227  0.5460  0.1872  0.0068 -0.1480
                                    -0.0531 -0.0312  0.7559  0.2618 -0.0041
                                     0.0025 -0.0044 -0.0010 -0.0011
312. (0.00091) RY*( 3) C   7        s(  0.20%)p99.99( 92.84%)d34.38(  6.96%)
                                     0.0000  0.0008 -0.0286  0.0347 -0.0006
                                     0.0044  0.5296 -0.1162  0.0062  0.7419
                                    -0.1529 -0.0022 -0.2385  0.0604  0.0595
                                    -0.0965 -0.0404  0.2314  0.0398
313. (0.00054) RY*( 4) C   7        s( 31.82%)p 0.04(  1.17%)d 2.11( 67.00%)
                                     0.0000 -0.0007  0.5641  0.0036  0.0053
                                    -0.0105 -0.0432  0.0786 -0.0005  0.0217
                                     0.0498  0.0078  0.0114 -0.0205  0.3133
                                     0.2650  0.5326  0.3620 -0.2949
314. (0.00051) RY*( 5) C   7        s( 67.58%)p 0.02(  1.28%)d 0.46( 31.14%)
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                                      0.0000 -0.0006  0.8061  0.1611  0.0026
                                     -0.0052 -0.0323 -0.0059  0.0126  0.0744
                                     -0.0677  0.0057  0.0158 -0.0336 -0.1973
                                     -0.1567 -0.3885 -0.2305  0.2095
315. (0.00020) RY*( 6) C   7        s(  0.09%)p99.99( 33.18%)d99.99( 66.72%)
                                      0.0000  0.0015 -0.0072  0.0289 -0.0039
                                     -0.0187  0.1082 -0.2940  0.0046 -0.0339
                                      0.0531 -0.0270  0.1434 -0.4562 -0.3354
                                      0.1460 -0.3243  0.2072 -0.6208
316. (0.00007) RY*( 7) C   7        s( 29.40%)p 1.36( 40.10%)d 1.04( 30.50%)
317. (0.00004) RY*( 8) C   7        s(  1.01%)p33.02( 33.42%)d64.79( 65.57%)
318. (0.00005) RY*( 9) C   7        s(  6.51%)p10.07( 65.60%)d 4.28( 27.88%)
319. (0.00004) RY*(10) C   7        s( 20.16%)p 2.65( 53.44%)d 1.31( 26.40%)
320. (0.00001) RY*(11) C   7        s( 37.76%)p 1.46( 55.28%)d 0.18(  6.97%)
321. (0.00000) RY*(12) C   7        s(  2.81%)p 8.08( 22.71%)d26.51( 74.48%)
322. (0.00000) RY*(13) C   7        s(  3.05%)p 3.19(  9.72%)d28.61( 87.23%)
323. (0.00000) RY*(14) C   7        s( 98.59%)p 0.01(  0.53%)d 0.01(  0.88%)
324. (0.00422) RY*( 1) C   8        s(  1.92%)p46.46( 89.25%)d 4.59(  8.83%)
                                      0.0000  0.0060  0.1383 -0.0070  0.0026
                                      0.0172  0.6836  0.0547 -0.0115 -0.4740
                                     -0.0416  0.0138  0.4265 -0.1157 -0.0779
                                      0.1418 -0.1728  0.0728 -0.1641
325. (0.00147) RY*( 2) C   8        s(  0.32%)p99.99( 97.86%)d 5.68(  1.82%)
                                      0.0000  0.0069  0.0550 -0.0098  0.0056
                                     -0.0037  0.4957 -0.0199  0.0139 -0.0414
                                     -0.1351  0.0209 -0.8432  0.0317  0.0561
                                      0.0166  0.0008  0.0953  0.0752
326. (0.00131) RY*( 3) C   8        s(  0.06%)p99.99( 93.97%)d95.04(  5.96%)
                                      0.0000  0.0004 -0.0137  0.0197  0.0073
                                     -0.0068 -0.3968  0.1978  0.0050 -0.8045
                                      0.1538  0.0148 -0.2515 -0.0935 -0.0564
                                      0.0696  0.0551 -0.2183  0.0300
327. (0.00060) RY*( 4) C   8        s( 92.45%)p 0.05(  4.59%)d 0.03(  2.97%)
                                      0.0000 -0.0007  0.9514 -0.1387 -0.0079
                                     -0.0107 -0.1389 -0.0277  0.0016  0.0693
                                     -0.0578 -0.0200 -0.0114 -0.1304  0.1266
                                      0.0815  0.0421 -0.0653  0.0306
328. (0.00046) RY*( 5) C   8        s(  0.66%)p 9.49(  6.28%)d99.99( 93.06%)
                                      0.0000  0.0005  0.0799 -0.0132 -0.0071
                                     -0.0063 -0.1360 -0.0360 -0.0055 -0.1563
                                     -0.1322  0.0026  0.0177 -0.0261 -0.0914
                                     -0.5626 -0.5355  0.4397  0.3544
329. (0.00016) RY*( 6) C   8        s(  5.18%)p 9.27( 48.08%)d 9.01( 46.74%)
                                      0.0000 -0.0071  0.1748  0.1435 -0.0252
                                     -0.0101  0.0402 -0.4083  0.0111 -0.0302
                                      0.4742  0.0094 -0.1000  0.2762 -0.4040
                                     -0.3329 -0.0043 -0.0608 -0.4355
330. (0.00012) RY*( 7) C   8        s(  4.04%)p10.55( 42.63%)d13.19( 53.33%)
                                      0.0000 -0.0095  0.0686  0.1858  0.0332
                                     -0.0002  0.1424 -0.1116 -0.0047 -0.0230
                                      0.4283 -0.0182  0.0914  0.4482  0.1460
                                      0.2264 -0.1061 -0.1614  0.6506
331. (0.00008) RY*( 8) C   8        s(  6.28%)p 9.23( 57.92%)d 5.70( 35.80%)
332. (0.00005) RY*( 9) C   8        s( 16.98%)p 0.93( 15.83%)d 3.96( 67.19%)
333. (0.00004) RY*(10) C   8        s(  0.87%)p99.99( 90.77%)d 9.65(  8.36%)
334. (0.00002) RY*(11) C   8        s(  1.58%)p 8.56( 13.53%)d53.72( 84.89%)
335. (0.00002) RY*(12) C   8        s( 24.34%)p 1.53( 37.16%)d 1.58( 38.50%)
336. (0.00002) RY*(13) C   8        s( 48.12%)p 0.05(  2.23%)d 1.03( 49.65%)
337. (0.00000) RY*(14) C   8        s( 97.23%)p 0.00(  0.04%)d 0.03(  2.73%)
338. (0.00631) RY*( 1) N   9        s(  0.08%)p99.99( 99.07%)d11.12(  0.85%)
                                      0.0000 -0.0029  0.0271  0.0050  0.0008
                                     -0.0117  0.7015 -0.0053  0.0042 -0.2809
                                      0.0167 -0.0046  0.6472  0.0161  0.0485
                                      0.0289 -0.0416  0.0103 -0.0592
339. (0.00502) RY*( 2) N   9        s(  6.40%)p13.23( 84.72%)d 1.39(  8.87%)
                                      0.0000 -0.0039  0.2513 -0.0298  0.0010
                                     -0.0081  0.3050 -0.0189  0.0064 -0.5950
                                      0.0386  0.0076 -0.6309  0.0078  0.2447
                                      0.0918 -0.1167 -0.0803 -0.0183
340. (0.00155) RY*( 3) N   9        s(  0.24%)p99.99( 87.77%)d49.36( 11.99%)
                                      0.0000  0.0034  0.0486 -0.0073 -0.0008
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                                      0.0116  0.5509  0.0328  0.0115  0.6787
                                      0.0942 -0.0038 -0.3209 -0.0193  0.1739
                                     -0.0490 -0.0348  0.2915  0.0321
341. (0.00096) RY*( 4) N   9          s( 82.79%)p 0.08(  6.62%)d 0.13( 10.59%)
                                      0.0000  0.0055  0.9088  0.0449 -0.0014
                                     -0.0025 -0.1539 -0.0068 -0.0036  0.0945
                                      0.0692 -0.0083  0.1682  0.0186 -0.1312
                                     -0.0880 -0.2546  0.1116  0.0608
342. (0.00073) RY*( 5) N   9          s(  7.33%)p 0.11(  0.83%)d12.53( 91.83%)
                                      0.0000  0.0017  0.2620  0.0684  0.0011
                                      0.0082 -0.0144 -0.0405  0.0057  0.0657
                                     -0.0388 -0.0005  0.0202  0.0131  0.0730
                                      0.5953  0.6947  0.0413 -0.2725
343. (0.00052) RY*( 6) N   9          s(  0.90%)p17.15( 15.45%)d92.87( 83.65%)
                                      0.0000  0.0018  0.0679 -0.0663  0.0014
                                      0.0165  0.1695 -0.1089  0.0246  0.2774
                                     -0.1388 -0.0095 -0.0687  0.1097 -0.2219
                                      0.1727 -0.1883 -0.8372 -0.1455
344. (0.00038) RY*( 7) N   9          s(  2.31%)p 3.05(  7.03%)d39.32( 90.66%)
                                      0.0000  0.0001  0.1200  0.0929  0.0048
                                      0.0095  0.0380  0.1207 -0.0004  0.0234
                                     -0.0829  0.0014  0.0471  0.2112  0.2871
                                     -0.2611  0.4250 -0.3063  0.6940
345. (0.00016) RY*( 8) N   9          s(  0.13%)p99.99( 30.31%)d99.99( 69.56%)
                                      0.0000 -0.0008 -0.0213  0.0280  0.0052
                                      0.0057  0.1928  0.2448 -0.0038 -0.1133
                                      0.0069 -0.0113 -0.1852  0.3983 -0.7851
                                     -0.0590  0.1947  0.1669  0.0997
346. (0.00013) RY*( 9) N   9          s( 19.33%)p 2.74( 53.01%)d 1.43( 27.66%)
                                      0.0000  0.0084 -0.0735  0.4332 -0.0138
                                     -0.0095 -0.0830  0.1801  0.0023  0.0359
                                     -0.3633 -0.0031  0.0423  0.5964  0.2580
                                      0.2810 -0.3329  0.1372 -0.0374
347. (0.00008) RY*(10) N   9          s( 24.73%)p 1.76( 43.41%)d 1.29( 31.85%)
348. (0.00006) RY*(11) N   9          s( 17.94%)p 4.03( 72.38%)d 0.54(  9.68%)
349. (0.00004) RY*(12) N   9          s( 36.31%)p 0.35( 12.55%)d 1.41( 51.15%)
350. (0.00004) RY*(13) N   9          s(  1.63%)p53.20( 86.93%)d 7.00( 11.44%)
351. (0.00000) RY*(14) N   9          s( 99.93%)p 0.00(  0.02%)d 0.00(  0.06%)
352. (0.00546) RY*( 1) C  10          s(  2.87%)p30.92( 88.75%)d 2.92(  8.38%)
                                      0.0000  0.0191  0.1498  0.0763  0.0087
                                     -0.0323 -0.5458  0.0398 -0.0080 -0.5751
                                      0.0938 -0.0207  0.4909 -0.0776 -0.1045
                                      0.1253  0.2389 -0.0016  0.0076
353. (0.00341) RY*( 2) C  10          s( 24.58%)p 1.68( 41.26%)d 1.39( 34.16%)
                                      0.0000 -0.0119  0.4577 -0.1901 -0.0057
                                     -0.0108  0.3851 -0.1683 -0.0003  0.2261
                                      0.0616 -0.0348  0.4169  0.0773  0.3217
                                      0.2137  0.3950  0.1844  0.0494
354. (0.00210) RY*( 3) C  10          s( 13.16%)p 6.19( 81.42%)d 0.41(  5.42%)
                                      0.0000 -0.0054  0.3550 -0.0740 -0.0088
                                     -0.0195  0.4076  0.1868  0.0279 -0.4997
                                     -0.4994  0.0194 -0.1353 -0.3069 -0.0963
                                     -0.0080 -0.1619  0.1195 -0.0662
355. (0.00162) RY*( 4) C  10          s( 37.93%)p 1.01( 38.34%)d 0.63( 23.73%)
                                      0.0000  0.0005  0.5704 -0.2322  0.0027
                                     -0.0035 -0.2807 -0.4851 -0.0265  0.0721
                                      0.0221  0.0226 -0.1293  0.2137 -0.1928
                                     -0.0411 -0.4024 -0.1129 -0.1541
356. (0.00138) RY*( 5) C  10          s(  5.24%)p13.90( 72.87%)d 4.18( 21.89%)
                                      0.0000  0.0032  0.2281 -0.0185 -0.0024
                                     -0.0152 -0.3366  0.3327 -0.0009  0.0306
                                     -0.2737  0.0051 -0.4857  0.4390  0.1494
                                      0.1158  0.3596  0.1878  0.1363
357. (0.00126) RY*( 6) C  10          s(  0.94%)p74.80( 70.56%)d30.21( 28.50%)
                                      0.0000 -0.0022 -0.0107  0.0955 -0.0141
                                      0.0008  0.2786 -0.2208 -0.0022 -0.5078
                                      0.3909 -0.0009 -0.3430  0.2256  0.2969
                                      0.1500  0.0990 -0.4028  0.0485
358. (0.00112) RY*( 7) C  10          s(  1.79%)p10.41( 18.66%)d44.37( 79.55%)
                                      0.0000 -0.0021 -0.0687  0.1149  0.0018
                                      0.0084  0.1210  0.2477 -0.0028 -0.0030
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                                     0.1590 -0.0043  0.0603  0.2856 -0.1751
                                     0.5916 -0.2258  0.2115 -0.5649
359. (0.00064) RY*( 8) C  10       s( 24.42%)p 2.88( 70.24%)d 0.22(  5.34%)
                                     0.0000 -0.0119  0.4638  0.1701  0.0066
                                    -0.0051 -0.0473  0.5249 -0.0163  0.1914
                                     0.5024 -0.0011 -0.1132 -0.3500  0.0309
                                    -0.0355 -0.1311 -0.1569  0.0966
360. (0.00036) RY*( 9) C  10       s( 81.90%)p 0.18( 14.54%)d 0.04(  3.56%)
                                     0.0000  0.0003  0.1640  0.8897 -0.0212
                                    -0.0048  0.0130 -0.2202 -0.0138  0.1198
                                    -0.2701  0.0067  0.0809  0.0509  0.0738
                                     0.0854 -0.0921 -0.0393  0.1134
361. (0.00014) RY*(10) C  10       s(  3.29%)p 6.24( 20.51%)d23.19( 76.20%)
                                     0.0000 -0.0086  0.1050  0.1444 -0.0301
                                    -0.0083  0.2915  0.0210  0.0075 -0.0283
                                     0.1854  0.0093  0.0000  0.2903 -0.7350
                                    -0.3116  0.3456  0.0357  0.0637
362. (0.00014) RY*(11) C  10       s(  1.59%)p12.92( 20.58%)d48.87( 77.83%)
                                     0.0000  0.0011 -0.0221  0.1068  0.0635
                                    -0.0098 -0.0078 -0.1703  0.0171 -0.1974
                                     0.3472  0.0052 -0.1293 -0.0065  0.1390
                                    -0.1868 -0.2015  0.8082  0.1741
363. (0.00008) RY*(12) C  10       s(  0.71%)p83.87( 59.33%)d56.49( 39.96%)
364. (0.00004) RY*(13) C  10       s(  2.89%)p 1.10(  3.17%)d32.46( 93.93%)
365. (0.00001) RY*(14) C  10       s( 98.66%)p 0.00(  0.10%)d 0.01(  1.24%)
366. (0.00639) RY*( 1) N  11       s(  0.05%)p99.99( 99.23%)d14.18(  0.72%)
                                     0.0000  0.0020  0.0116  0.0192 -0.0003
                                     0.0029 -0.4746 -0.0097  0.0046 -0.1187
                                     0.0139  0.0064 -0.8675 -0.0003 -0.0638
                                     0.0200 -0.0345 -0.0343 -0.0193
367. (0.00514) RY*( 2) N  11       s(  6.11%)p13.83( 84.48%)d 1.54(  9.41%)
                                     0.0000 -0.0040  0.2321 -0.0848 -0.0001
                                     0.0040 -0.4106  0.0238 -0.0137  0.8151
                                    -0.0306 -0.0029  0.0969 -0.0280  0.1128
                                    -0.0712 -0.1061  0.2506  0.0473
368. (0.00167) RY*( 3) N  11       s(  1.24%)p69.25( 86.09%)d10.19( 12.66%)
                                     0.0000  0.0040  0.1011 -0.0469 -0.0008
                                     0.0117  0.7185  0.0952  0.0088  0.3569
                                     0.0119 -0.0063 -0.4505 -0.0697  0.2820
                                     0.1370 -0.1278 -0.0583 -0.0929
369. (0.00107) RY*( 4) N  11       s( 86.36%)p 0.08(  7.21%)d 0.07(  6.43%)
                                     0.0000  0.0053  0.9231  0.1068  0.0011
                                    -0.0082 -0.0201  0.0081  0.0020 -0.2562
                                    -0.0446 -0.0007  0.0527 -0.0342  0.1426
                                     0.0191 -0.0141 -0.1422  0.1523
370. (0.00067) RY*( 5) N  11       s(  3.45%)p 0.40(  1.38%)d27.62( 95.18%)
                                     0.0000  0.0013  0.1751  0.0615  0.0017
                                     0.0073  0.0649 -0.0702  0.0048 -0.0110
                                    -0.0554 -0.0050 -0.0327  0.0154 -0.2539
                                     0.4688  0.4783  0.5382 -0.3862
371. (0.00051) RY*( 6) N  11       s(  1.00%)p15.64( 15.59%)d83.67( 83.41%)
                                     0.0000  0.0014  0.0948  0.0313  0.0004
                                     0.0256  0.2832 -0.1339  0.0109  0.0710
                                    -0.1010 -0.0121 -0.1677  0.1160 -0.4858
                                    -0.5432  0.1749  0.2907  0.4336
372. (0.00037) RY*( 7) N  11       s(  2.71%)p 2.71(  7.34%)d33.19( 89.95%)
                                     0.0000  0.0008  0.1101  0.1223  0.0052
                                     0.0037  0.0575  0.0486  0.0047 -0.0128
                                    -0.0505  0.0011  0.0453  0.2509 -0.4966
                                     0.0969 -0.7423  0.0680 -0.2963
373. (0.00015) RY*( 8) N  11       s( 49.14%)p 0.77( 37.60%)d 0.27( 13.26%)
                                     0.0000  0.0049 -0.1127  0.6919 -0.0028
                                    -0.0056 -0.0126 -0.1574 -0.0003  0.0921
                                    -0.1193 -0.0038 -0.0144  0.5728  0.2618
                                     0.1513  0.0512 -0.0019  0.1963
374. (0.00014) RY*( 9) N  11       s(  1.48%)p18.31( 27.07%)d48.31( 71.45%)
                                     0.0000  0.0016 -0.0440  0.1133  0.0005
                                     0.0006  0.0177 -0.3315 -0.0119 -0.2639
                                     0.1806  0.0035 -0.0109 -0.2408  0.4183
                                    -0.2177 -0.3289  0.6174 -0.0521
375. (0.00010) RY*(10) N  11       s( 18.28%)p 3.46( 63.26%)d 1.01( 18.46%)
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                                      0.0000  0.0008 -0.0286  0.4266  0.0063
                                      0.0036  0.0135 -0.4764  0.0062  0.1842
                                      0.0756  0.0078  0.0176 -0.6045 -0.2751
                                      0.1638 -0.0225 -0.2775  0.0675
376. (0.00006) RY*(11) N  11        s( 18.05%)p 4.33( 78.17%)d 0.21(  3.77%)
377. (0.00004) RY*(12) N  11        s(  6.90%)p13.10( 90.45%)d 0.38(  2.64%)
378. (0.00005) RY*(13) N  11        s(  5.31%)p 0.42(  2.20%)d17.43( 92.49%)
379. (0.00000) RY*(14) N  11        s( 99.97%)p 0.00(  0.01%)d 0.00(  0.02%)
380. (0.00425) RY*( 1) C  12        s(  0.75%)p99.99( 82.83%)d21.81( 16.41%)
                                      0.0000 -0.0014  0.0844 -0.0201 -0.0009
                                      0.0102  0.3445 -0.0881 -0.0007 -0.1711
                                      0.0231  0.0197  0.7763 -0.2626 -0.1020
                                     -0.2016 -0.3036 -0.1188  0.0827
381. (0.00301) RY*( 2) C  12        s(  8.61%)p 9.21( 79.35%)d 1.40( 12.04%)
                                      0.0000 -0.0070  0.2933 -0.0012  0.0059
                                     -0.0141 -0.7487  0.0178 -0.0068  0.2759
                                      0.1564  0.0077  0.3601  0.0457 -0.0570
                                     -0.1562 -0.0217  0.3019  0.0329
382. (0.00144) RY*( 3) C  12        s(  2.58%)p35.30( 90.91%)d 2.53(  6.52%)
                                      0.0000 -0.0043  0.1457 -0.0670  0.0043
                                     -0.0038  0.3350 -0.0841 -0.0436  0.8303
                                      0.3053 -0.0045  0.0431  0.0589  0.0983
                                      0.1046  0.0332 -0.2061 -0.0315
383. (0.00111) RY*( 4) C  12        s( 61.90%)p 0.55( 34.34%)d 0.06(  3.77%)
                                      0.0000  0.0065  0.7859 -0.0296 -0.0187
                                      0.0119  0.1178 -0.3911  0.0034 -0.1710
                                     -0.1723 -0.0003 -0.1785  0.2926 -0.1547
                                     -0.0073 -0.0859 -0.0681 -0.0410
384. (0.00070) RY*( 5) C  12        s(  2.06%)p 6.20( 12.80%)d41.23( 85.13%)
                                      0.0000  0.0025  0.1429 -0.0150 -0.0016
                                     -0.0020  0.1051 -0.1599  0.0043 -0.0883
                                     -0.1133 -0.0084  0.2403 -0.1138  0.3732
                                      0.0840  0.7891  0.1454  0.2473
385. (0.00041) RY*( 6) C  12        s( 10.61%)p 7.96( 84.42%)d 0.47(  4.97%)
                                      0.0000 -0.0065  0.3224  0.0415  0.0195
                                      0.0146  0.0015  0.6849 -0.0073  0.1679
                                     -0.5637 -0.0054  0.0379 -0.1656  0.0859
                                      0.0339 -0.0036 -0.1902 -0.0704
386. (0.00027) RY*( 7) C  12        s( 16.61%)p 4.48( 74.49%)d 0.54(  8.89%)
                                      0.0000  0.0145 -0.2191  0.3392 -0.0536
                                     -0.0025 -0.1831 -0.5166 -0.0009  0.2777
                                     -0.5598 -0.0001  0.0245 -0.2313 -0.0819
                                      0.2138 -0.1260 -0.0922  0.1102
387. (0.00016) RY*( 8) C  12        s(  6.84%)p12.59( 86.16%)d 1.02(  6.99%)
                                      0.0000 -0.0084  0.2543 -0.0294  0.0535
                                      0.0066 -0.0971 -0.0665 -0.0007 -0.0848
                                      0.3017 -0.0035 -0.2480 -0.8295 -0.0967
                                      0.1594  0.0367 -0.0562 -0.1752
388. (0.00011) RY*( 9) C  12        s(  2.00%)p 2.09(  4.19%)d46.81( 93.81%)
                                      0.0000 -0.0026 -0.0417  0.1337  0.0203
                                     -0.0066  0.1141  0.1382 -0.0315  0.0921
                                      0.0074 -0.0022 -0.0026  0.0123 -0.8612
                                     -0.0904  0.3903  0.0259  0.1880
389. (0.00012) RY*(10) C  12        s( 42.16%)p 0.49( 20.71%)d 0.88( 37.13%)
                                      0.0000 -0.0024  0.0484  0.6461  0.0424
                                      0.0067 -0.1716  0.0693  0.0046 -0.1812
                                      0.2833 -0.0015  0.1559  0.1880  0.0656
                                      0.1790  0.1405 -0.5373 -0.1629
390. (0.00004) RY*(11) C  12        s( 41.68%)p 0.27( 11.31%)d 1.13( 47.01%)
391. (0.00002) RY*(12) C  12        s(  0.53%)p16.63(  8.77%)d99.99( 90.70%)
392. (0.00002) RY*(13) C  12        s(  4.81%)p 1.84(  8.84%)d17.94( 86.34%)
393. (0.00000) RY*(14) C  12        s( 98.91%)p 0.01(  1.00%)d 0.00(  0.09%)
394. (0.00426) RY*( 1) C  13        s(  0.82%)p99.99( 82.67%)d20.24( 16.52%)
                                      0.0000 -0.0022  0.0847 -0.0313 -0.0021
                                      0.0114  0.3047 -0.1219 -0.0043 -0.1714
                                      0.1075  0.0185  0.7912 -0.2270  0.0450
                                     -0.2355 -0.1246 -0.2021  0.2265
395. (0.00304) RY*( 2) C  13        s(  8.63%)p 9.22( 79.62%)d 1.36( 11.74%)
                                      0.0000 -0.0068  0.2937  0.0025  0.0055
                                     -0.0115 -0.0976  0.1333 -0.0125 -0.8549
                                     -0.0477  0.0052 -0.1809 -0.0524  0.1863
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                                      0.1266 -0.0272 -0.2415 -0.0872
396. (0.00151) RY*( 3) C  13          s(  1.51%)p61.64( 92.89%)d 3.72(  5.60%)
                                      0.0000  0.0046 -0.0593  0.1073  0.0022
                                      0.0374 -0.8611 -0.1954 -0.0130  0.0542
                                      0.1354 -0.0213  0.3198  0.1537  0.1290
                                      0.0613  0.0140 -0.1874 -0.0177
397. (0.00109) RY*( 4) C  13          s( 64.80%)p 0.48( 31.20%)d 0.06(  4.00%)
                                      0.0000  0.0059  0.8046 -0.0212 -0.0130
                                      0.0070 -0.0277 -0.2161  0.0092  0.2306
                                     -0.4049  0.0046 -0.0108  0.2172 -0.0462
                                     -0.1151  0.0802 -0.0555  0.1228
398. (0.00069) RY*( 5) C  13          s(  3.48%)p 3.70( 12.87%)d24.03( 83.65%)
                                      0.0000  0.0009  0.1862 -0.0112  0.0038
                                      0.0002  0.0745 -0.2168  0.0043 -0.0424
                                      0.0689 -0.0088  0.2634 -0.0106 -0.2932
                                      0.4474 -0.2445  0.2845 -0.6401
399. (0.00044) RY*( 6) C  13          s(  7.15%)p12.07( 86.27%)d 0.92(  6.58%)
                                      0.0000 -0.0061  0.2651  0.0286  0.0187
                                      0.0010  0.1045 -0.1462  0.0156 -0.0635
                                      0.8271  0.0058 -0.1455  0.3477 -0.0298
                                     -0.1816  0.0779  0.1373  0.0840
400. (0.00024) RY*( 7) C  13          s(  6.02%)p13.96( 84.05%)d 1.65(  9.93%)
                                      0.0000  0.0103 -0.1180  0.2101 -0.0451
                                      0.0004 -0.0021 -0.7847 -0.0004 -0.1599
                                     -0.0475 -0.0034 -0.2410 -0.3727 -0.0787
                                      0.0651  0.0577  0.1352  0.2593
401. (0.00015) RY*( 8) C  13          s( 11.23%)p 6.98( 78.41%)d 0.92( 10.35%)
                                      0.0000 -0.0142  0.3168 -0.0812  0.0719
                                     -0.0022 -0.1885  0.2451  0.0077  0.2061
                                      0.2761  0.0037 -0.0678 -0.7518 -0.1082
                                      0.0199  0.2877 -0.0494 -0.0788
402. (0.00012) RY*( 9) C  13          s( 59.57%)p 0.19( 11.56%)d 0.48( 28.88%)
                                      0.0000 -0.0031  0.0108  0.7716  0.0134
                                     -0.0023 -0.0517  0.2481  0.0062 -0.1545
                                     -0.1044  0.0028  0.1227  0.0383 -0.3828
                                     -0.2383  0.1991  0.2126 -0.0243
403. (0.00009) RY*(10) C  13          s(  1.30%)p 4.82(  6.29%)d70.81( 92.40%)
404. (0.00005) RY*(11) C  13          s( 30.10%)p 0.52( 15.61%)d 1.80( 54.29%)
405. (0.00002) RY*(12) C  13          s(  2.97%)p 2.55(  7.59%)d30.08( 89.44%)
406. (0.00002) RY*(13) C  13          s(  3.44%)p 2.98( 10.28%)d25.04( 86.27%)
407. (0.00000) RY*(14) C  13          s( 99.03%)p 0.01(  0.81%)d 0.00(  0.16%)
408. (0.00292) RY*( 1) B  14          s(  9.96%)p 8.81( 87.77%)d 0.23(  2.27%)
                                      0.0000  0.0098  0.3144  0.0072  0.0252
                                      0.0117 -0.8196 -0.2924  0.0085 -0.3067
                                     -0.1500 -0.0023 -0.0586  0.0158 -0.0056
                                      0.1186  0.0611  0.0609 -0.0343
409. (0.00140) RY*( 2) B  14          s(  3.39%)p20.72( 70.23%)d 7.79( 26.39%)
                                      0.0000 -0.0024  0.1594  0.0751 -0.0533
                                     -0.0036  0.2298 -0.1893 -0.0042 -0.2324
                                      0.1146  0.0056  0.6056 -0.4238  0.0581
                                      0.2952  0.2519  0.2168 -0.2508
410. (0.00130) RY*( 3) B  14          s(  1.47%)p65.49( 96.10%)d 1.66(  2.43%)
                                      0.0000  0.0009  0.0815  0.0896  0.0020
                                     -0.0057  0.3424 -0.1709  0.0104 -0.7053
                                      0.2972  0.0044 -0.4441  0.1773 -0.0360
                                     -0.0552  0.0664  0.1198  0.0351
411. (0.00095) RY*( 4) B  14          s( 64.43%)p 0.46( 29.93%)d 0.09(  5.65%)
                                      0.0000 -0.0128  0.7969  0.0939 -0.0178
                                      0.0037  0.1725  0.1029 -0.0009  0.3951
                                      0.0761  0.0066 -0.3114  0.0028  0.0014
                                      0.1794  0.1033  0.0732 -0.0907
412. (0.00063) RY*( 5) B  14          s(  5.85%)p15.55( 90.94%)d 0.55(  3.21%)
                                      0.0000 -0.0182 -0.0312  0.2361 -0.0381
                                     -0.0174 -0.2875  0.7554 -0.0008 -0.1522
                                      0.4514 -0.0076  0.1196  0.1204  0.0665
                                      0.0856  0.0631  0.0528 -0.1166
413. (0.00045) RY*( 6) B  14          s( 36.37%)p 0.88( 31.99%)d 0.87( 31.64%)
                                      0.0000 -0.0022 -0.3156  0.5126 -0.0366
                                     -0.0061  0.0155 -0.2199  0.0044  0.2010
                                     -0.1462 -0.0036 -0.0928  0.4482  0.0468
                                      0.3068  0.3342  0.0762 -0.3202
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414. (0.00038) RY*( 7) B  14          s( 20.53%)p 3.72( 76.42%)d 0.15(  3.05%)
                                        0.0000 -0.0027 -0.2201  0.3942 -0.0384
                                        0.0027 -0.1025  0.0297 -0.0098  0.0587
                                       -0.0211  0.0003 -0.4471 -0.7409  0.0119
                                       -0.1124  0.0038  0.0176 -0.1320
415. (0.00037) RY*( 8) B  14          s(  1.63%)p53.16( 86.80%)d 7.09( 11.57%)
                                        0.0000 -0.0012  0.0882  0.0755 -0.0534
                                        0.0130  0.1451  0.4278 -0.0245 -0.2733
                                       -0.7668 -0.0108  0.0046  0.0161 -0.1667
                                       -0.0146  0.0260  0.2947  0.0116
416. (0.00019) RY*( 9) B  14          s( 52.64%)p 0.21( 11.26%)d 0.69( 36.10%)
                                        0.0000  0.0063  0.2217  0.6811 -0.1154
                                       -0.0107  0.0519 -0.1195 -0.0034 -0.0587
                                       -0.0420  0.0097  0.2915  0.0722  0.1112
                                       -0.2050 -0.3568 -0.2155  0.3645
417. (0.00013) RY*(10) B  14          s(  1.36%)p 8.43( 11.46%)d64.11( 87.18%)
                                        0.0000 -0.0006 -0.0604  0.0889 -0.0451
                                        0.0131 -0.0760 -0.1306 -0.0200  0.1845
                                        0.2228 -0.0036  0.0653  0.0569 -0.5866
                                       -0.0932 -0.3128  0.6487  0.0202
418. (0.00009) RY*(11) B  14          s( 16.70%)p 0.17(  2.83%)d 4.82( 80.47%)
419. (0.00007) RY*(12) B  14          s( 58.94%)p 0.02(  1.26%)d 0.68( 39.80%)
420. (0.00004) RY*(13) B  14          s( 25.43%)p 0.03(  0.65%)d 2.91( 73.92%)
421. (0.00004) RY*(14) B  14          s(  1.39%)p 1.86(  2.57%)d69.33( 96.04%)
422. (0.00328) RY*( 1) B  15          s( 40.38%)p 1.22( 49.18%)d 0.26( 10.44%)
                                        0.0000  0.0063  0.6343  0.0314  0.0209
                                        0.0056  0.5981  0.1782  0.0026  0.2376
                                        0.1433 -0.0032 -0.0672 -0.1444  0.0649
                                       -0.2918 -0.1135 -0.0400  0.0226
423. (0.00182) RY*( 2) B  15          s(  4.47%)p17.82( 79.64%)d 3.56( 15.89%)
                                        0.0000 -0.0241  0.1756  0.1065 -0.0439
                                        0.0019  0.0293 -0.5263  0.0055 -0.1107
                                       -0.3854 -0.0188  0.5030  0.3231  0.0759
                                       -0.3732 -0.0717 -0.0856 -0.0378
424. (0.00127) RY*( 3) B  15          s(  0.33%)p99.99( 96.16%)d10.50(  3.51%)
                                        0.0000  0.0008  0.0266  0.0501 -0.0109
                                        0.0084 -0.3324 -0.0349 -0.0065  0.8399
                                       -0.2839 -0.0144 -0.2275  0.1087  0.0163
                                       -0.1253  0.0335  0.0738 -0.1119
425. (0.00122) RY*( 4) B  15          s(  4.05%)p23.00( 93.13%)d 0.70(  2.82%)
                                        0.0000  0.0019  0.1903 -0.0637  0.0142
                                       -0.0069  0.0046 -0.0150  0.0166 -0.3105
                                       -0.0693 -0.0149 -0.6540  0.6337  0.0551
                                       -0.0537  0.0450 -0.0282 -0.1396
426. (0.00116) RY*( 5) B  15          s( 30.44%)p 2.25( 68.49%)d 0.04(  1.07%)
                                        0.0000 -0.0146  0.5434  0.0851 -0.0411
                                       -0.0055 -0.6062 -0.2168 -0.0045 -0.2371
                                        0.1078  0.0165 -0.1548 -0.4223  0.0415
                                       -0.0732 -0.0209  0.0556  0.0073
427. (0.00070) RY*( 6) B  15          s( 21.47%)p 3.51( 75.48%)d 0.14(  3.05%)
                                        0.0000  0.0042  0.3546 -0.2927  0.0575
                                       -0.0046 -0.3091  0.5999 -0.0144 -0.0195
                                       -0.0851 -0.0052  0.4305  0.3258 -0.0770
                                        0.1534 -0.0314 -0.0029 -0.0036
428. (0.00037) RY*( 7) B  15          s(  9.45%)p 2.23( 21.11%)d 7.35( 69.44%)
                                        0.0000  0.0045  0.2969  0.0794 -0.0033
                                        0.0081  0.1903 -0.2524 -0.0109  0.0812
                                       -0.3211 -0.0054 -0.0149 -0.0323  0.0147
                                        0.8066  0.1078 -0.1658  0.0664
429. (0.00028) RY*( 8) B  15          s( 12.94%)p 2.01( 25.96%)d 4.72( 61.10%)
                                        0.0000  0.0067  0.1224  0.3329 -0.0591
                                       -0.0081 -0.0004 -0.1255  0.0237  0.0939
                                        0.3616  0.0081  0.1040  0.3046 -0.3438
                                        0.0558  0.3439  0.4670  0.3916
430. (0.00024) RY*( 9) B  15          s( 74.84%)p 0.24( 17.71%)d 0.10(  7.45%)
                                        0.0000  0.0009 -0.0442  0.8590 -0.0927
                                        0.0127 -0.0674  0.3822 -0.0069 -0.0977
                                       -0.1227  0.0026  0.0212  0.0349  0.1735
                                        0.0018 -0.0536 -0.1867 -0.0816
431. (0.00017) RY*(10) B  15          s(  0.98%)p66.88( 65.45%)d34.30( 33.57%)
                                        0.0000  0.0001 -0.0237 -0.0396  0.0875
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                                     0.0007  0.0986  0.2255 -0.0002 -0.2033
                                    -0.6809  0.0028 -0.1533 -0.2558 -0.1782
                                    -0.1948  0.2331  0.3130  0.3372
432. (0.00009) RY*(11) B  15       s( 24.56%)p 0.14(  3.34%)d 2.94( 72.10%)
433. (0.00006) RY*(12) B  15       s( 66.86%)p 0.02(  1.52%)d 0.47( 31.62%)
434. (0.00005) RY*(13) B  15       s(  7.62%)p 0.14(  1.05%)d11.99( 91.34%)
435. (0.00003) RY*(14) B  15       s(  1.73%)p 1.07(  1.86%)d55.85( 96.42%)
436. (0.00549) RY*( 1) C  16       s(  2.24%)p41.31( 92.37%)d 2.41(  5.39%)
                                     0.0000  0.0206  0.0790  0.1247  0.0121
                                     0.0222  0.6832 -0.0792  0.0080  0.6009
                                    -0.1050 -0.0211 -0.2772  0.0288 -0.1876
                                     0.1151 -0.0123  0.0074  0.0724
437. (0.00277) RY*( 2) C  16       s( 28.97%)p 1.78( 51.67%)d 0.67( 19.36%)
                                     0.0000 -0.0087  0.5181 -0.1454  0.0080
                                     0.0071 -0.1147  0.3833 -0.0112  0.3265
                                    -0.1112 -0.0387  0.4850  0.0280 -0.2426
                                    -0.3335 -0.1455  0.0433  0.0227
438. (0.00260) RY*( 3) C  16       s( 13.29%)p 5.31( 70.55%)d 1.22( 16.16%)
                                     0.0000 -0.0023  0.3522 -0.0938  0.0050
                                    -0.0149  0.4285  0.4083  0.0437 -0.4829
                                     0.0378 -0.0074 -0.0694  0.3372  0.2339
                                     0.1710 -0.0062 -0.1996  0.1944
439. (0.00186) RY*( 4) C  16       s( 28.13%)p 2.48( 69.86%)d 0.07(  2.00%)
                                     0.0000 -0.0024  0.5083 -0.1513 -0.0073
                                     0.0309 -0.3442 -0.0135  0.0079  0.1344
                                     0.3091  0.0151 -0.6541 -0.1931  0.0472
                                    -0.0167 -0.0372 -0.1270 -0.0041
440. (0.00133) RY*( 5) C  16       s(  6.41%)p 7.59( 48.62%)d 7.02( 44.98%)
                                     0.0000 -0.0015  0.2388 -0.0833 -0.0088
                                     0.0111  0.3627 -0.2105 -0.0015 -0.3063
                                     0.3580 -0.0018  0.1418 -0.2609 -0.2453
                                    -0.0837  0.1305  0.2109 -0.5666
441. (0.00128) RY*( 6) C  16       s(  4.51%)p 7.19( 32.45%)d13.98( 63.04%)
                                     0.0000 -0.0011  0.1908 -0.0927 -0.0097
                                     0.0092  0.0676 -0.1348  0.0050  0.1238
                                     0.1387  0.0138  0.2999 -0.4206  0.4406
                                     0.2437  0.3141  0.2996  0.4342
442. (0.00081) RY*( 7) C  16       s( 16.87%)p 3.25( 54.78%)d 1.68( 28.34%)
                                     0.0000 -0.0106  0.3825  0.1488 -0.0136
                                     0.0074 -0.0883 -0.3068  0.0090 -0.0527
                                    -0.6562  0.0000  0.0750 -0.0823  0.1551
                                     0.2512  0.1229 -0.2864 -0.3149
443. (0.00077) RY*( 8) C  16       s( 18.69%)p 2.63( 49.13%)d 1.72( 32.18%)
                                     0.0000 -0.0083  0.2866  0.3234 -0.0086
                                     0.0061 -0.0512 -0.5113 -0.0014 -0.1637
                                     0.0226 -0.0078 -0.0286  0.4461 -0.1261
                                    -0.3293  0.0969  0.2635  0.3445
444. (0.00044) RY*( 9) C  16       s( 73.93%)p 0.28( 20.42%)d 0.08(  5.65%)
                                     0.0000  0.0027  0.0413  0.8588 -0.0035
                                     0.0013 -0.0086  0.2912  0.0078 -0.0163
                                     0.2020 -0.0017  0.0475 -0.2755  0.0704
                                    -0.1107  0.0536 -0.1900 -0.0198
445. (0.00019) RY*(10) C  16       s(  1.13%)p28.00( 31.76%)d59.16( 67.11%)
                                     0.0000  0.0018  0.0084  0.1010 -0.0326
                                     0.0189 -0.1367  0.3567 -0.0079  0.1467
                                    -0.1078  0.0148 -0.1862  0.3213  0.1813
                                     0.0812  0.4460  0.5544 -0.3539
446. (0.00013) RY*(11) C  16       s(  4.92%)p 1.83(  9.01%)d17.49( 86.07%)
                                     0.0000 -0.0084  0.1128  0.1625 -0.1001
                                     0.0072 -0.2070  0.0276  0.0038 -0.0388
                                     0.1456  0.0038  0.1156  0.1016 -0.4632
                                     0.7515 -0.2086  0.1753  0.0844
447. (0.00008) RY*(12) C  16       s(  0.04%)p99.99( 68.09%)d99.99( 31.87%)
448. (0.00004) RY*(13) C  16       s(  2.30%)p 0.67(  1.54%)d41.90( 96.16%)
449. (0.00001) RY*(14) C  16       s( 98.53%)p 0.00(  0.12%)d 0.01(  1.35%)
450. (0.00554) RY*( 1) N  17       s(  5.76%)p14.80( 85.26%)d 1.56(  8.99%)
                                     0.0000 -0.0042  0.2247 -0.0841 -0.0004
                                    -0.0062  0.4138 -0.0290  0.0095 -0.3984
                                    -0.0005 -0.0147  0.7220 -0.0106  0.1665
                                    -0.1190  0.1390  0.1242 -0.1150
451. (0.00483) RY*( 2) N  17       s(  0.38%)p99.99( 98.01%)d 4.22(  1.61%)
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                                     0.0000  0.0007  0.0615 -0.0057 -0.0003
                                    -0.0034  0.3447  0.0120  0.0048 -0.6943
                                     0.0020  0.0070 -0.6156 -0.0007 -0.0384
                                    -0.0193  0.0242 -0.0113 -0.1163
452. (0.00166) RY*( 3) N  17        s(  0.27%)p99.99( 92.92%)d25.30(  6.81%)
                                     0.0000  0.0044  0.0414 -0.0309 -0.0003
                                    -0.0140 -0.7997 -0.1335 -0.0100 -0.5050
                                    -0.0366  0.0041  0.1223 -0.0120  0.1209
                                    -0.2048 -0.0534 -0.0933 -0.0011
453. (0.00121) RY*( 4) N  17        s( 90.75%)p 0.06(  5.46%)d 0.04(  3.79%)
                                     0.0000  0.0060  0.9475  0.0985  0.0013
                                     0.0068 -0.0454 -0.0395 -0.0072  0.1698
                                     0.0100  0.0025 -0.1431 -0.0378  0.0345
                                    -0.0460  0.0258 -0.1430  0.1162
454. (0.00075) RY*( 5) N  17        s(  0.64%)p 2.23(  1.43%)d99.99( 97.92%)
                                     0.0000  0.0004  0.0753  0.0277  0.0006
                                    -0.0074 -0.0522  0.0559  0.0000 -0.0143
                                    -0.0380  0.0058  0.0000 -0.0821 -0.6058
                                    -0.4131 -0.0424  0.6403  0.1728
455. (0.00065) RY*( 6) N  17        s(  1.23%)p 9.24( 11.34%)d71.23( 87.43%)
                                     0.0000  0.0014  0.1095  0.0164  0.0015
                                    -0.0253 -0.2309  0.1759 -0.0174 -0.0979
                                     0.1357  0.0027  0.0041 -0.0131 -0.0408
                                     0.6979  0.4447  0.4229 -0.0951
456. (0.00032) RY*( 7) N  17        s(  0.90%)p 1.94(  1.74%)d99.99( 97.37%)
                                     0.0000  0.0000  0.0738  0.0591  0.0045
                                    -0.0056 -0.0693 -0.0101  0.0039  0.0801
                                    -0.0116  0.0101  0.0704 -0.0282 -0.4384
                                    -0.0176 -0.0240 -0.2153 -0.8569
457. (0.00014) RY*( 8) N  17        s(  0.15%)p73.97( 11.19%)d99.99( 88.66%)
                                     0.0000 -0.0009  0.0040  0.0377  0.0087
                                     0.0019  0.0512 -0.0452 -0.0092 -0.2222
                                     0.0658  0.0082  0.2272  0.0414 -0.5944
                                     0.3875 -0.2009 -0.4243  0.4035
458. (0.00014) RY*( 9) N  17        s( 62.68%)p 0.45( 27.96%)d 0.15(  9.36%)
                                     0.0000  0.0055 -0.0896  0.7866 -0.0033
                                     0.0029 -0.0075  0.3874  0.0006 -0.0603
                                     0.3465 -0.0022  0.0604  0.0459  0.0384
                                    -0.2047  0.1763 -0.1298  0.0479
459. (0.00010) RY*(10) N  17        s(  0.46%)p99.99( 97.69%)d 4.05(  1.86%)
460. (0.00005) RY*(11) N  17        s( 26.19%)p 2.68( 70.23%)d 0.14(  3.58%)
461. (0.00005) RY*(12) N  17        s(  5.75%)p 0.54(  3.13%)d15.85( 91.12%)
462. (0.00004) RY*(13) N  17        s(  4.96%)p18.89( 93.78%)d 0.25(  1.26%)
463. (0.00000) RY*(14) N  17        s( 99.92%)p 0.00(  0.01%)d 0.00(  0.07%)
464. (0.00366) RY*( 1) C  18        s(  0.01%)p 1.00( 84.57%)d 0.18( 15.42%)
                                     0.0000  0.0010  0.0053  0.0059  0.0019
                                     0.0051  0.2317 -0.0148 -0.0128 -0.6379
                                     0.1981 -0.0141 -0.5460  0.2174 -0.0851
                                    -0.1770 -0.0165  0.2239  0.2554
465. (0.00314) RY*( 2) C  18        s(  9.39%)p 8.44( 79.29%)d 1.21( 11.32%)
                                     0.0000 -0.0063  0.3062 -0.0101  0.0060
                                     0.0163  0.8138 -0.0156  0.0108  0.0021
                                    -0.1062 -0.0030  0.3290  0.1021  0.0868
                                     0.0472  0.1541  0.2266 -0.1683
466. (0.00146) RY*( 3) C  18        s(  1.03%)p89.42( 91.82%)d 6.97(  7.15%)
                                     0.0000  0.0032 -0.0482  0.0890 -0.0029
                                     0.0022  0.2158 -0.1212 -0.0299  0.6062
                                     0.1893  0.0324 -0.6402 -0.2045  0.0301
                                     0.0459  0.1327  0.1790 -0.1373
467. (0.00107) RY*( 4) C  18        s( 63.84%)p 0.50( 31.93%)d 0.07(  4.23%)
                                     0.0000  0.0057  0.7978 -0.0390 -0.0185
                                    -0.0119 -0.1923  0.4223 -0.0008  0.0288
                                     0.3025  0.0027 -0.1069  0.0089 -0.1059
                                     0.0966 -0.0458 -0.0923 -0.1054
468. (0.00069) RY*( 5) C  18        s(  2.97%)p 3.82( 11.36%)d28.82( 85.67%)
                                     0.0000  0.0010  0.1719 -0.0125  0.0004
                                    -0.0014 -0.0730  0.0507 -0.0082  0.2036
                                    -0.0309 -0.0052  0.1503 -0.2015  0.2202
                                    -0.0511  0.0871  0.3626  0.8164
469. (0.00044) RY*( 6) C  18        s(  9.86%)p 8.40( 82.83%)d 0.74(  7.31%)
                                     0.0000 -0.0084  0.3119  0.0281  0.0215
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                                    -0.0170 -0.0041 -0.7933  0.0016 -0.1190
                                     0.2810 -0.0054  0.1002 -0.3090  0.0038
                                    -0.0380 -0.2055 -0.1699  0.0232
470. (0.00024) RY*( 7) C  18       s( 11.08%)p 7.16( 79.35%)d 0.86(  9.57%)
                                     0.0000  0.0155 -0.2130  0.2496 -0.0542
                                     0.0027  0.2275  0.3480  0.0004 -0.2093
                                     0.2619 -0.0015  0.1156 -0.7035 -0.1597
                                    -0.0609  0.1393 -0.2142  0.0342
471. (0.00016) RY*( 8) C  18       s(  7.15%)p11.97( 85.60%)d 1.01(  7.25%)
                                     0.0000 -0.0084  0.2541  0.0611  0.0562
                                    -0.0067  0.0066 -0.0197 -0.0004 -0.1038
                                    -0.8032 -0.0015 -0.2698 -0.3560 -0.2204
                                    -0.0224 -0.1521 -0.0088 -0.0153
472. (0.00011) RY*( 9) C  18       s(  0.38%)p12.63(  4.79%)d99.99( 94.83%)
                                     0.0000  0.0016  0.0531 -0.0213 -0.0229
                                    -0.0023  0.1028  0.1476 -0.0223  0.0772
                                    -0.0499  0.0233 -0.0772 -0.0123  0.5707
                                    -0.6843 -0.2700 -0.2775 -0.0662
473. (0.00009) RY*(10) C  18       s( 33.08%)p 0.64( 21.23%)d 1.38( 45.69%)
474. (0.00002) RY*(11) C  18       s( 16.47%)p 0.56(  9.27%)d 4.51( 74.26%)
475. (0.00003) RY*(12) C  18       s(  8.89%)p 0.92(  8.18%)d 9.33( 82.93%)
476. (0.00003) RY*(13) C  18       s( 36.93%)p 0.24(  9.01%)d 1.46( 54.06%)
477. (0.00000) RY*(14) C  18       s( 98.98%)p 0.01(  0.90%)d 0.00(  0.12%)
478. (0.00371) RY*( 1) C  19       s(  0.52%)p99.99( 84.10%)d29.63( 15.38%)
                                     0.0000 -0.0036  0.0688 -0.0208 -0.0020
                                    -0.0033 -0.1957  0.0562  0.0164  0.7217
                                    -0.2397  0.0120  0.4546 -0.1191  0.2271
                                     0.2092  0.0267 -0.2370 -0.0393
479. (0.00308) RY*( 2) C  19       s(  9.42%)p 8.41( 79.20%)d 1.21( 11.38%)
                                     0.0000 -0.0068  0.3067 -0.0089  0.0047
                                     0.0116 -0.0629 -0.1432  0.0105  0.4473
                                     0.0128 -0.0098 -0.7530  0.0009 -0.0002
                                    -0.1698 -0.1971 -0.1794  0.1181
480. (0.00145) RY*( 3) C  19       s(  1.34%)p68.68( 92.07%)d 4.91(  6.59%)
                                     0.0000  0.0030 -0.0758  0.0874 -0.0022
                                    -0.0422  0.8875  0.2465 -0.0024  0.1726
                                    -0.0824 -0.0134  0.0595  0.1735  0.0044
                                    -0.0879 -0.1294 -0.1739  0.1054
481. (0.00096) RY*( 4) C  19       s( 70.69%)p 0.39( 27.47%)d 0.03(  1.83%)
                                     0.0000  0.0054  0.8405 -0.0154 -0.0148
                                    -0.0059  0.0741  0.2844 -0.0078 -0.1017
                                     0.3524  0.0093  0.1974 -0.1213 -0.0846
                                     0.0987 -0.0104  0.0328 -0.0158
482. (0.00064) RY*( 5) C  19       s(  0.32%)p48.50( 15.76%)d99.99( 83.91%)
                                     0.0000 -0.0030  0.0437 -0.0360  0.0061
                                     0.0024 -0.1039  0.1408 -0.0086  0.1847
                                    -0.2341 -0.0024  0.1465  0.1285 -0.5844
                                    -0.4759 -0.1994  0.2184 -0.4286
483. (0.00048) RY*( 6) C  19       s(  6.07%)p13.32( 80.82%)d 2.16( 13.11%)
                                     0.0000 -0.0093  0.2422 -0.0411  0.0157
                                     0.0016 -0.1299  0.2840 -0.0080 -0.1340
                                    -0.5294  0.0149 -0.1344  0.6278  0.2321
                                     0.1662  0.1228  0.1763  0.0588
484. (0.00025) RY*( 7) C  19       s( 10.53%)p 7.78( 81.89%)d 0.72(  7.58%)
                                     0.0000 -0.0150  0.2544 -0.1905  0.0635
                                    -0.0033  0.1689 -0.7940 -0.0019 -0.0587
                                    -0.0481  0.0034  0.2593  0.2950  0.1048
                                    -0.0288 -0.2429  0.0390 -0.0589
485. (0.00014) RY*( 8) C  19       s(  3.55%)p26.13( 92.79%)d 1.03(  3.65%)
                                     0.0000 -0.0074  0.1819 -0.0342  0.0347
                                     0.0014  0.1646 -0.1093 -0.0031 -0.2057
                                    -0.6689  0.0009 -0.0697 -0.6279 -0.1007
                                     0.0860 -0.0221  0.0849  0.1063
486. (0.00011) RY*( 9) C  19       s(  8.78%)p 0.65(  5.72%)d 9.73( 85.49%)
                                     0.0000 -0.0044 -0.0437  0.2902  0.0411
                                     0.0288 -0.0968 -0.0875  0.0028  0.0243
                                    -0.0154  0.0094  0.0435  0.1912 -0.6254
                                     0.5200 -0.2088 -0.1262  0.3659
487. (0.00010) RY*(10) C  19       s( 42.48%)p 0.29( 12.31%)d 1.06( 45.21%)
488. (0.00005) RY*(11) C  19       s( 35.64%)p 0.36( 12.78%)d 1.45( 51.59%)
489. (0.00002) RY*(12) C  19       s( 11.04%)p 0.67(  7.42%)d 7.39( 81.54%)
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490. (0.00003) RY*(13) C  19          s(  0.43%)p16.77(  7.17%)d99.99( 92.40%)
491. (0.00000) RY*(14) C  19          s( 99.25%)p 0.01(  0.62%)d 0.00(  0.13%)
492. (0.00571) RY*( 1) N  20          s(  5.93%)p14.59( 86.49%)d 1.28(  7.59%)
                                        0.0000 -0.0043  0.2302 -0.0791 -0.0006
                                        0.0165 -0.7529  0.0031 -0.0061  0.4907
                                       -0.0197  0.0045 -0.2369  0.0209  0.0994
                                       -0.2150 -0.0624 -0.1245 -0.0193
493. (0.00498) RY*( 2) N  20          s(  1.16%)p82.40( 95.77%)d 2.64(  3.06%)
                                        0.0000 -0.0005  0.1042 -0.0276  0.0002
                                       -0.0004 -0.0128 -0.0048  0.0064 -0.5359
                                       -0.0072  0.0123 -0.8185  0.0113  0.1191
                                       -0.0637  0.0110 -0.0767  0.0799
494. (0.00169) RY*( 3) N  20          s(  2.89%)p29.88( 86.33%)d 3.73( 10.78%)
                                        0.0000  0.0039  0.1679 -0.0261 -0.0014
                                       -0.0111 -0.4772 -0.0237 -0.0110 -0.6387
                                       -0.1102  0.0047  0.4546  0.0892  0.1503
                                       -0.1268  0.1482  0.1504 -0.1568
495. (0.00108) RY*( 4) N  20          s( 84.86%)p 0.12( 10.35%)d 0.06(  4.79%)
                                        0.0000  0.0057  0.9125  0.1258  0.0022
                                       -0.0013  0.2990  0.0091  0.0067  0.1044
                                        0.0073 -0.0107  0.0285  0.0450  0.0155
                                        0.0444  0.1858  0.0203 -0.1038
496. (0.00071) RY*( 5) N  20          s(  2.14%)p 0.88(  1.88%)d44.94( 95.98%)
                                        0.0000  0.0012  0.1337  0.0591  0.0000
                                       -0.0054 -0.0124  0.0674 -0.0055 -0.0531
                                        0.0026  0.0034  0.0513 -0.0928 -0.3902
                                       -0.4361 -0.1709  0.3880  0.6615
497. (0.00059) RY*( 6) N  20          s(  2.76%)p 5.28( 14.61%)d29.90( 82.63%)
                                        0.0000  0.0022  0.1563  0.0565  0.0016
                                       -0.0166 -0.1126  0.1241 -0.0214 -0.2148
                                        0.2013  0.0133  0.1679 -0.0474 -0.3431
                                        0.1931 -0.3877 -0.7061  0.1494
498. (0.00032) RY*( 7) N  20          s(  0.06%)p38.29(  2.20%)d99.99( 97.74%)
                                        0.0000 -0.0006  0.0229 -0.0069  0.0009
                                       -0.0063 -0.0540 -0.0024  0.0034  0.0342
                                        0.0550  0.0057  0.1148 -0.0402  0.5780
                                        0.3647  0.2040 -0.1017  0.6770
499. (0.00014) RY*( 8) N  20          s( 74.34%)p 0.20( 15.22%)d 0.14( 10.44%)
                                        0.0000  0.0055 -0.1416  0.8505 -0.0022
                                        0.0028 -0.1037  0.1889  0.0022  0.0054
                                        0.3148 -0.0021 -0.0391 -0.0714  0.0136
                                       -0.1277  0.2886 -0.0414 -0.0536
500. (0.00015) RY*( 9) N  20          s(  0.10%)p99.99( 13.81%)d99.99( 86.09%)
                                        0.0000  0.0007 -0.0044  0.0304 -0.0097
                                        0.0119  0.2761  0.0786  0.0023  0.0006
                                       -0.0946  0.0059  0.1340 -0.1690  0.5291
                                       -0.6301 -0.3196 -0.2796 -0.0602
501. (0.00009) RY*(10) N  20          s(  1.26%)p74.43( 94.02%)d 3.74(  4.72%)
502. (0.00006) RY*(11) N  20          s( 12.83%)p 6.35( 81.47%)d 0.44(  5.70%)
503. (0.00004) RY*(12) N  20          s(  5.44%)p17.17( 93.44%)d 0.20(  1.11%)
504. (0.00004) RY*(13) N  20          s(  6.39%)p 0.70(  4.49%)d13.94( 89.11%)
505. (0.00000) RY*(14) N  20          s( 99.88%)p 0.00(  0.03%)d 0.00(  0.09%)
506. (0.00680) RY*( 1) C  21          s(  6.19%)p14.04( 86.94%)d 1.11(  6.86%)
                                        0.0000  0.0060  0.2377  0.0733 -0.0035
                                       -0.0145  0.5127  0.0304  0.0087 -0.4612
                                       -0.0132 -0.0126  0.6261  0.0182 -0.0376
                                        0.1233 -0.2276  0.0142 -0.0019
507. (0.00357) RY*( 2) C  21          s(  0.05%)p99.99( 96.76%)d67.94(  3.19%)
                                        0.0000 -0.0035  0.0158 -0.0130 -0.0062
                                       -0.0002 -0.8216 -0.0068 -0.0053 -0.3432
                                        0.0336  0.0001  0.4090 -0.0792 -0.0785
                                        0.0883  0.0394  0.0847 -0.0962
508. (0.00291) RY*( 3) C  21          s(  0.06%)p99.99( 90.61%)d99.99(  9.32%)
                                        0.0000  0.0024  0.0224  0.0116  0.0004
                                       -0.0044  0.0124  0.0072  0.0022 -0.7532
                                        0.0372  0.0082 -0.5806 -0.0065  0.1458
                                        0.1322  0.0327  0.0787  0.2173
509. (0.00116) RY*( 4) C  21          s( 34.42%)p 1.62( 55.87%)d 0.28(  9.71%)
                                        0.0000 -0.0052  0.5857  0.0290  0.0164
                                       -0.0083 -0.1269  0.2483  0.0023  0.0474
                                       -0.4787 -0.0007 -0.0393  0.4979  0.0324
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                                    -0.2223  0.1118  0.1051  0.1519
510. (0.00089) RY*( 5) C  21          s( 26.65%)p 0.92( 24.65%)d 1.83( 48.70%)
                                      0.0000  0.0009 -0.1903  0.4799  0.0058
                                     -0.0077 -0.0070  0.3572  0.0020  0.0212
                                     -0.3418 -0.0039  0.0178 -0.0349  0.2679
                                      0.4562  0.1933 -0.3636 -0.1938
511. (0.00078) RY*( 6) C  21          s( 39.45%)p 0.22(  8.82%)d 1.31( 51.73%)
                                      0.0000  0.0027 -0.3646  0.5114 -0.0017
                                      0.0071 -0.0044  0.2144  0.0118  0.0263
                                     -0.1366 -0.0014  0.0666 -0.1350 -0.0992
                                     -0.2739 -0.1727  0.5208  0.3625
512. (0.00068) RY*( 7) C  21          s( 19.49%)p 3.18( 61.96%)d 0.95( 18.56%)
                                      0.0000 -0.0020 -0.2521  0.3623  0.0018
                                      0.0000 -0.0182 -0.2125 -0.0034 -0.1291
                                      0.2374 -0.0081 -0.0536  0.7058 -0.1912
                                     -0.1490 -0.1128 -0.1183 -0.3163
513. (0.00043) RY*( 8) C  21          s( 10.99%)p 5.45( 59.91%)d 2.65( 29.09%)
                                      0.0000 -0.0002  0.1247  0.3072 -0.0054
                                     -0.0088 -0.0827 -0.6970 -0.0040 -0.0001
                                     -0.2693  0.0062  0.0378 -0.1801  0.3470
                                     -0.2288 -0.1438 -0.2659  0.1638
514. (0.00039) RY*( 9) C  21          s( 28.62%)p 0.87( 24.89%)d 1.62( 46.49%)
                                      0.0000  0.0030  0.4108  0.3428  0.0036
                                      0.0042  0.0268  0.0781 -0.0068 -0.0571
                                      0.0460 -0.0097 -0.2306 -0.4282 -0.3235
                                     -0.2406 -0.0149  0.0409 -0.5481
515. (0.00036) RY*(10) C  21          s( 28.13%)p 1.55( 43.55%)d 1.01( 28.32%)
                                      0.0000  0.0027  0.3877  0.3619  0.0036
                                     -0.0007 -0.0385 -0.0367  0.0048  0.2096
                                      0.6190  0.0045  0.0367  0.0640  0.3023
                                      0.2694  0.1837  0.2229  0.1893
516. (0.00014) RY*(11) C  21          s(  2.77%)p 3.61(  9.99%)d31.55( 87.24%)
                                      0.0000 -0.0057  0.1637  0.0248  0.0142
                                     -0.0128 -0.1586  0.0100  0.0142  0.1786
                                     -0.0614 -0.0160 -0.1923  0.0372 -0.2066
                                      0.4538 -0.7824 -0.0368  0.1012
517. (0.00010) RY*(12) C  21          s(  0.19%)p99.99( 33.98%)d99.99( 65.83%)
                                      0.0000 -0.0017  0.0352  0.0197 -0.0164
                                     -0.0032 -0.1033  0.4542 -0.0014 -0.0547
                                      0.3383  0.0004  0.0336 -0.0655  0.1374
                                     -0.4390 -0.2483 -0.5700  0.2452
518. (0.00005) RY*(13) C  21          s(  3.38%)p 0.64(  2.16%)d27.98( 94.46%)
519. (0.00000) RY*(14) C  21          s( 99.66%)p 0.00(  0.04%)d 0.00(  0.30%)
520. (0.00535) RY*( 1) C  22          s(  0.51%)p99.99( 93.02%)d12.60(  6.47%)
                                      0.0000  0.0018  0.0289  0.0652 -0.0070
                                     -0.0108  0.2486 -0.0206  0.0194 -0.7813
                                      0.0516  0.0122 -0.5042  0.0062 -0.1289
                                     -0.0204 -0.0041 -0.0381 -0.2149
521. (0.00398) RY*( 2) C  22          s(  4.41%)p20.77( 91.62%)d 0.90(  3.97%)
                                      0.0000 -0.0064  0.2022 -0.0563 -0.0012
                                     -0.0069 -0.6975 -0.0712 -0.0062 -0.5012
                                     -0.1016 -0.0002  0.4030  0.0247 -0.0575
                                     -0.0577  0.0834  0.1429  0.0757
522. (0.00332) RY*( 3) C  22          s(  6.57%)p12.92( 84.87%)d 1.30(  8.56%)
                                      0.0000  0.0007  0.2563  0.0005  0.0030
                                     -0.0089  0.6097  0.0430 -0.0004 -0.2209
                                      0.0368  0.0051  0.6517 -0.0102  0.0489
                                     -0.1980  0.1678 -0.1230  0.0270
523. (0.00190) RY*( 4) C  22          s( 86.02%)p 0.13( 11.00%)d 0.03(  2.97%)
                                      0.0000 -0.0027  0.9273 -0.0175 -0.0007
                                     -0.0046 -0.0453 -0.0177 -0.0155  0.1814
                                      0.0508  0.0016 -0.2376  0.1243  0.0383
                                      0.0775 -0.0899 -0.1161 -0.0265
524. (0.00075) RY*( 5) C  22          s(  0.79%)p63.07( 49.97%)d62.14( 49.23%)
                                      0.0000 -0.0060  0.0825  0.0313  0.0099
                                      0.0095  0.0592 -0.3776 -0.0009  0.0181
                                      0.0353  0.0081  0.0691 -0.5892  0.0073
                                      0.5777  0.2996  0.1627 -0.2057
525. (0.00047) RY*( 6) C  22          s(  1.83%)p36.13( 66.07%)d17.56( 32.10%)
                                      0.0000 -0.0030  0.0054  0.1325  0.0263
                                      0.0081 -0.0096 -0.4489  0.0046  0.0679
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                                    0.6694  0.0063  0.0713 -0.0353 -0.2687
                                   -0.3120 -0.2972  0.2496 -0.0300
526. (0.00045) RY*( 7) C  22      s( 22.15%)p 1.95( 43.11%)d 1.57( 34.74%)
                                    0.0000  0.0052 -0.0656  0.4660  0.0008
                                   -0.0034 -0.0514 -0.0950  0.0053  0.0278
                                    0.2434 -0.0084  0.0158  0.5992  0.1964
                                    0.2005  0.4990  0.0412 -0.1340
527. (0.00033) RY*( 8) C  22      s( 69.23%)p 0.35( 24.41%)d 0.09(  6.37%)
                                    0.0000  0.0001  0.0592  0.8299 -0.0098
                                    0.0033 -0.0951  0.2858 -0.0091  0.0001
                                   -0.0840  0.0052  0.0376 -0.3805  0.0599
                                   -0.1206 -0.1945 -0.0877 -0.0030
528. (0.00028) RY*( 9) C  22      s(  2.50%)p 6.28( 15.68%)d32.74( 81.82%)
                                    0.0000  0.0019  0.1246  0.0955  0.0188
                                    0.0147  0.1776  0.1904  0.0029  0.0801
                                   -0.2642 -0.0081 -0.0936  0.0612 -0.3667
                                   -0.0811  0.1978  0.7772  0.1842
529. (0.00014) RY*(10) C  22      s(  0.25%)p90.73( 22.90%)d99.99( 76.85%)
                                    0.0000 -0.0007  0.0341 -0.0294 -0.0223
                                   -0.0052 -0.0865 -0.2545  0.0067  0.0982
                                   -0.0842 -0.0146 -0.2577 -0.2708  0.1740
                                   -0.6271  0.5650 -0.1200  0.1058
530. (0.00013) RY*(11) C  22      s(  0.08%)p99.99( 10.69%)d99.99( 89.24%)
                                    0.0000 -0.0026  0.0023  0.0217  0.0173
                                    0.0010  0.0851 -0.0469 -0.0070 -0.1825
                                    0.2143 -0.0109 -0.1196 -0.0610  0.4157
                                    0.1934 -0.0692  0.1112  0.8155
531. (0.00008) RY*(12) C  22      s(  4.15%)p20.41( 84.64%)d 2.70( 11.21%)
532. (0.00004) RY*(13) C  22      s(  1.81%)p 1.12(  2.04%)d53.11( 96.15%)
533. (0.00000) RY*(14) C  22      s( 99.72%)p 0.00(  0.13%)d 0.00(  0.16%)
534. (0.00409) RY*( 1) C  23      s(  1.83%)p48.80( 89.18%)d 4.92(  8.99%)
                                    0.0000  0.0051  0.1349 -0.0072  0.0027
                                   -0.0001  0.0664  0.0540  0.0097  0.2980
                                   -0.1151  0.0240  0.8828  0.0491  0.1462
                                   -0.0201  0.1144  0.0508  0.2291
535. (0.00148) RY*( 2) C  23      s(  0.03%)p99.99( 97.90%)d62.27(  2.07%)
                                    0.0000  0.0065 -0.0092  0.0127  0.0067
                                   -0.0159 -0.0861  0.1681  0.0155 -0.9117
                                    0.0936 -0.0040  0.3195  0.0283 -0.0200
                                   -0.1288 -0.0078 -0.0602  0.0051
536. (0.00141) RY*( 3) C  23      s(  2.11%)p44.20( 93.20%)d 2.23(  4.69%)
                                    0.0000  0.0016  0.1436 -0.0203  0.0071
                                   -0.0082  0.9190 -0.1511  0.0143 -0.1616
                                   -0.1670 -0.0068 -0.0317  0.0959 -0.0850
                                    0.1122  0.1104  0.0762 -0.0956
537. (0.00067) RY*( 4) C  23      s( 86.84%)p 0.07(  5.67%)d 0.09(  7.49%)
                                    0.0000 -0.0004  0.9197 -0.1499 -0.0070
                                    0.0052 -0.0849  0.1611 -0.0170  0.0033
                                   -0.0471 -0.0129 -0.1380 -0.0419  0.1006
                                   -0.1507 -0.0491 -0.1915 -0.0550
538. (0.00046) RY*( 5) C  23      s(  5.05%)p 1.36(  6.85%)d17.46( 88.10%)
                                    0.0000 -0.0001  0.2246 -0.0012  0.0000
                                   -0.0033 -0.2163 -0.1216 -0.0104 -0.0625
                                   -0.0539 -0.0011  0.0012  0.0042 -0.3611
                                    0.0268  0.2350  0.8313 -0.0607
539. (0.00015) RY*( 6) C  23      s(  5.74%)p 8.95( 51.40%)d 7.47( 42.86%)
                                    0.0000 -0.0082  0.1779  0.1582 -0.0255
                                   -0.0106  0.0304 -0.4017  0.0093 -0.1001
                                    0.3480 -0.0124  0.0583 -0.4657  0.1234
                                    0.4389 -0.3608  0.0813  0.2898
540. (0.00011) RY*( 7) C  23      s(  6.63%)p 4.94( 32.75%)d 9.15( 60.62%)
                                    0.0000 -0.0088  0.0787  0.2442  0.0191
                                    0.0090 -0.0891 -0.4447 -0.0163  0.0425
                                    0.2717 -0.0023  0.1646 -0.1370 -0.2254
                                   -0.0777  0.4720 -0.3499 -0.4519
541. (0.00009) RY*( 8) C  23      s(  9.35%)p 6.55( 61.20%)d 3.15( 29.45%)
542. (0.00005) RY*( 9) C  23      s( 16.43%)p 1.05( 17.24%)d 4.04( 66.32%)
543. (0.00003) RY*(10) C  23      s(  0.46%)p99.99( 86.90%)d27.51( 12.64%)
544. (0.00003) RY*(11) C  23      s( 63.04%)p 0.16( 10.03%)d 0.43( 26.92%)
545. (0.00002) RY*(12) C  23      s(  1.38%)p12.05( 16.63%)d59.44( 81.99%)
546. (0.00002) RY*(13) C  23      s(  4.44%)p 6.97( 30.92%)d14.58( 64.65%)
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547. (0.00000) RY*(14) C  23          s( 96.71%)p 0.00(  0.29%)d 0.03(  3.00%)
548. (0.00400) RY*( 1) C  24          s(  1.02%)p89.09( 90.72%)d 8.12(  8.27%)
                                        0.0000  0.0005  0.0910  0.0433  0.0057
                                        0.0144  0.4540 -0.0256 -0.0170 -0.5718
                                        0.0327  0.0228  0.6082 -0.0379 -0.0184
                                        0.1392 -0.2467  0.0401 -0.0216
549. (0.00185) RY*( 2) C  24          s(  0.03%)p99.99( 99.85%)d 3.53(  0.12%)
                                        0.0000 -0.0002  0.0114  0.0142  0.0002
                                        0.0101 -0.2531 -0.0726 -0.0253  0.5672
                                        0.2059 -0.0276  0.7146  0.2300  0.0135
                                        0.0273 -0.0012 -0.0157  0.0003
550. (0.00092) RY*( 3) C  24          s(  0.18%)p99.99( 90.28%)d53.28(  9.54%)
                                        0.0000  0.0018  0.0310  0.0287  0.0005
                                       -0.0050 -0.7765  0.1861 -0.0017 -0.4900
                                        0.1086  0.0003  0.1142 -0.0192 -0.0056
                                       -0.2457 -0.1539 -0.0720  0.0783
551. (0.00055) RY*( 4) C  24          s( 80.54%)p 0.02(  2.01%)d 0.22( 17.45%)
                                        0.0000 -0.0014  0.8898  0.1166  0.0075
                                       -0.0054  0.0549  0.0086  0.0091  0.0986
                                       -0.0079 -0.0115 -0.0687  0.0479 -0.1743
                                       -0.2763 -0.0695  0.2399  0.0731
552. (0.00048) RY*( 5) C  24          s( 18.12%)p 0.13(  2.39%)d 4.39( 79.48%)
                                        0.0000 -0.0001  0.4212  0.0618 -0.0032
                                       -0.0114 -0.1286  0.0031 -0.0005 -0.0722
                                       -0.0377 -0.0029 -0.0246  0.0025  0.3748
                                        0.5369  0.2316 -0.5350 -0.1622
553. (0.00020) RY*( 6) C  24          s(  0.07%)p99.99( 34.69%)d99.99( 65.24%)
                                        0.0000  0.0015  0.0124  0.0226 -0.0036
                                        0.0087 -0.0422  0.1717 -0.0212  0.1059
                                       -0.3749 -0.0238  0.1390 -0.3788  0.3722
                                        0.1126  0.0290  0.2088  0.6759
554. (0.00007) RY*( 7) C  24          s( 37.25%)p 0.98( 36.56%)d 0.70( 26.19%)
555. (0.00005) RY*( 8) C  24          s(  4.61%)p18.00( 83.04%)d 2.68( 12.35%)
556. (0.00004) RY*( 9) C  24          s(  1.06%)p22.74( 24.13%)d70.53( 74.81%)
557. (0.00004) RY*(10) C  24          s(  0.45%)p99.99( 65.52%)d74.91( 34.02%)
558. (0.00001) RY*(11) C  24          s( 52.15%)p 0.31( 16.29%)d 0.61( 31.56%)
559. (0.00000) RY*(12) C  24          s( 97.88%)p 0.01(  0.74%)d 0.01(  1.37%)
560. (0.00001) RY*(13) C  24          s(  6.40%)p 4.96( 31.74%)d 9.67( 61.86%)
561. (0.00000) RY*(14) C  24          s(  0.28%)p79.46( 22.17%)d99.99( 77.55%)
562. (0.00401) RY*( 1) C  25          s(  1.50%)p59.38( 89.34%)d 6.09(  9.16%)
                                        0.0000  0.0053  0.1206 -0.0214  0.0028
                                        0.0110  0.4291  0.0333 -0.0207 -0.7628
                                       -0.0539 -0.0089 -0.3270  0.1260 -0.0990
                                       -0.1168  0.1024 -0.0742 -0.2282
563. (0.00145) RY*( 2) C  25          s(  0.11%)p99.99( 98.42%)d12.77(  1.46%)
                                        0.0000  0.0073  0.0313  0.0047  0.0094
                                       -0.0056  0.3971  0.0173  0.0076 -0.1520
                                       -0.0980 -0.0280  0.8895  0.0366 -0.0058
                                        0.0194  0.0922  0.0416  0.0631
564. (0.00127) RY*( 3) C  25          s(  0.07%)p99.99( 92.17%)d99.99(  7.76%)
                                        0.0000 -0.0033  0.0208  0.0151  0.0004
                                        0.0119  0.7074 -0.2628  0.0059  0.5128
                                       -0.1449  0.0023 -0.2595  0.0285 -0.1161
                                        0.0668  0.0668  0.2341 -0.0208
565. (0.00061) RY*( 4) C  25          s( 90.64%)p 0.04(  3.50%)d 0.06(  5.85%)
                                        0.0000 -0.0008  0.9445 -0.1199 -0.0043
                                       -0.0072 -0.0344  0.0209  0.0104  0.1153
                                        0.0983  0.0192  0.0119  0.0990  0.1020
                                       -0.1840 -0.0481 -0.0129  0.1084
566. (0.00048) RY*( 5) C  25          s(  3.83%)p 1.68(  6.43%)d23.41( 89.74%)
                                        0.0000 -0.0001  0.1910 -0.0429  0.0025
                                        0.0064 -0.1979 -0.1163  0.0061 -0.0787
                                       -0.0627  0.0041 -0.0006  0.0367  0.0694
                                        0.7194  0.5108  0.2438 -0.2339
567. (0.00015) RY*( 6) C  25          s(  1.36%)p20.82( 28.41%)d51.46( 70.23%)
                                        0.0000 -0.0056  0.1160 -0.0011 -0.0123
                                       -0.0093  0.0366 -0.2169  0.0090 -0.0115
                                        0.3688 -0.0187  0.1173 -0.2919 -0.3558
                                        0.2734 -0.5214 -0.0923 -0.4696
568. (0.00008) RY*( 7) C  25          s(  1.65%)p39.36( 65.07%)d20.13( 33.28%)
569. (0.00006) RY*( 8) C  25          s( 21.87%)p 2.46( 53.82%)d 1.11( 24.31%)
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570. (0.00005) RY*( 9) C  25          s( 19.03%)p 2.48( 47.19%)d 1.78( 33.78%)
571. (0.00005) RY*(10) C  25          s( 12.87%)p 1.94( 24.99%)d 4.83( 62.15%)
572. (0.00002) RY*(11) C  25          s(  0.67%)p40.14( 26.95%)d99.99( 72.38%)
573. (0.00001) RY*(12) C  25          s(  1.07%)p27.50( 29.45%)d64.89( 69.48%)
574. (0.00002) RY*(13) C  25          s( 47.54%)p 0.72( 34.21%)d 0.38( 18.26%)
575. (0.00000) RY*(14) C  25          s( 97.81%)p 0.00(  0.21%)d 0.02(  1.99%)
576. (0.00511) RY*( 1) C  26          s(  0.88%)p99.99( 92.22%)d 7.82(  6.89%)
                                        0.0000  0.0005 -0.0414  0.0842 -0.0036
                                        0.0012 -0.1827  0.0080 -0.0110  0.5261
                                       -0.0126 -0.0224  0.7811 -0.0320  0.1019
                                        0.0521 -0.0218  0.0684  0.2252
577. (0.00300) RY*( 2) C  26          s(  0.60%)p99.99( 91.61%)d13.10(  7.80%)
                                        0.0000  0.0023  0.0771 -0.0015  0.0021
                                        0.0058  0.9315  0.0917 -0.0010  0.1550
                                        0.0537 -0.0026  0.1126 -0.0168 -0.0332
                                       -0.2631  0.0019  0.0347  0.0802
578. (0.00288) RY*( 3) C  26          s(  4.94%)p17.52( 86.54%)d 1.72(  8.52%)
                                        0.0000 -0.0013  0.2221  0.0066  0.0044
                                        0.0013  0.0467 -0.0441 -0.0048 -0.7572
                                       -0.0323 -0.0025  0.5345  0.0345  0.1016
                                       -0.0308  0.2574 -0.0870  0.0080
579. (0.00144) RY*( 4) C  26          s( 89.11%)p 0.09(  8.24%)d 0.03(  2.65%)
                                        0.0000 -0.0024  0.9434 -0.0323 -0.0048
                                       -0.0025 -0.0907  0.0600 -0.0013  0.1873
                                       -0.1425  0.0123 -0.0873  0.0862  0.0161
                                       -0.0040 -0.1249 -0.1028 -0.0064
580. (0.00075) RY*( 5) C  26          s(  5.56%)p 2.39( 13.31%)d14.58( 81.13%)
                                        0.0000 -0.0032  0.1784  0.1541  0.0073
                                       -0.0119 -0.0614 -0.2064 -0.0122 -0.0672
                                        0.2003  0.0069  0.0133 -0.2039 -0.4164
                                       -0.0621  0.0702  0.7931 -0.0052
581. (0.00052) RY*( 6) C  26          s( 24.38%)p 2.53( 61.78%)d 0.57( 13.84%)
                                        0.0000  0.0072 -0.0640  0.4895 -0.0004
                                       -0.0051 -0.0321  0.3459  0.0092  0.0214
                                       -0.6922 -0.0068 -0.0838 -0.1016  0.0616
                                       -0.1742  0.2797  0.1525 -0.0522
582. (0.00044) RY*( 7) C  26          s( 33.67%)p 1.12( 37.87%)d 0.85( 28.46%)
                                        0.0000 -0.0012  0.0938  0.5726  0.0064
                                        0.0165  0.1341 -0.1613 -0.0021 -0.0174
                                        0.2458  0.0039 -0.0774 -0.5173  0.2498
                                        0.4285 -0.0496 -0.1899  0.0083
583. (0.00028) RY*( 8) C  26          s( 29.52%)p 1.93( 56.96%)d 0.46( 13.52%)
                                        0.0000 -0.0012  0.0201  0.5427 -0.0164
                                       -0.0051 -0.1002  0.0415  0.0049  0.0630
                                        0.4634  0.0039 -0.0583  0.5793  0.0014
                                       -0.2812  0.2106 -0.1085 -0.0005
584. (0.00020) RY*( 9) C  26          s(  6.31%)p 1.26(  7.98%)d13.57( 85.70%)
                                        0.0000  0.0005 -0.0634  0.2431 -0.0042
                                       -0.0038 -0.0981 -0.0401 -0.0127 -0.2231
                                       -0.0791  0.0062  0.0627 -0.0917 -0.0659
                                       -0.4469 -0.7830 -0.0740  0.1855
585. (0.00013) RY*(10) C  26          s(  0.00%)p 1.00( 19.38%)d 4.16( 80.62%)
                                        0.0000 -0.0016  0.0020  0.0051 -0.0032
                                       -0.0062 -0.0771  0.1463  0.0112  0.1059
                                        0.1333  0.0041  0.1974 -0.3135 -0.3838
                                       -0.2364  0.0397 -0.3061 -0.7125
586. (0.00011) RY*(11) C  26          s(  4.82%)p 9.66( 46.56%)d10.09( 48.62%)
                                        0.0000 -0.0030 -0.0603  0.2110  0.0063
                                        0.0068  0.1971 -0.3081 -0.0010 -0.0092
                                       -0.3225  0.0112  0.1350  0.4575 -0.3149
                                        0.4722 -0.2619 -0.0036 -0.3090
587. (0.00009) RY*(12) C  26          s(  0.02%)p99.99( 75.33%)d99.99( 24.65%)
588. (0.00004) RY*(13) C  26          s(  0.49%)p 4.67(  2.31%)d99.99( 97.20%)
589. (0.00000) RY*(14) C  26          s( 99.72%)p 0.00(  0.05%)d 0.00(  0.22%)
590. (0.00369) RY*( 1) C  27          s(  7.32%)p11.63( 85.14%)d 1.03(  7.54%)
                                        0.0000  0.0043  0.2566  0.0852  0.0085
                                       -0.0168 -0.4806  0.0086  0.0023  0.1484
                                       -0.0246 -0.0255 -0.7709  0.0505 -0.0744
                                        0.2466 -0.0618  0.0701 -0.0172
591. (0.00170) RY*( 2) C  27          s(  9.77%)p 8.29( 80.99%)d 0.94(  9.24%)
                                        0.0000  0.0011  0.3032  0.0760  0.0074
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                                     0.0012 -0.4057  0.0502  0.0015 -0.7697
                                     0.0687 -0.0031  0.2112 -0.0323 -0.1825
                                    -0.0066  0.1495  0.0167  0.1908
592. (0.00140) RY*( 3) C  27        s(  6.28%)p11.20( 70.31%)d 3.73( 23.42%)
                                     0.0000  0.0085  0.2059  0.1414 -0.0183
                                    -0.0114 -0.4190  0.0113  0.0035  0.4713
                                     0.3076 -0.0012  0.4587  0.0091  0.0756
                                    -0.0225 -0.2119  0.3714  0.2123
593. (0.00074) RY*( 4) C  27        s( 15.75%)p 3.52( 55.41%)d 1.83( 28.84%)
                                     0.0000  0.0031  0.2708  0.2889 -0.0268
                                    -0.0003  0.2104 -0.5178  0.0087 -0.0945
                                     0.1880 -0.0027  0.0283  0.4434  0.3737
                                     0.2871 -0.0720 -0.2344  0.0782
594. (0.00059) RY*( 5) C  27        s( 22.77%)p 2.53( 57.61%)d 0.86( 19.62%)
                                     0.0000 -0.0025  0.4542  0.1460  0.0066
                                    -0.0101  0.5335  0.2296 -0.0085  0.0151
                                     0.4150 -0.0028 -0.1817 -0.1818 -0.1130
                                    -0.0455  0.2785  0.3216  0.0200
595. (0.00037) RY*( 6) C  27        s( 36.87%)p 1.44( 53.14%)d 0.27(  9.99%)
                                     0.0000 -0.0019  0.5484 -0.2597 -0.0197
                                    -0.0109  0.1544  0.0906  0.0037  0.0260
                                    -0.6557 -0.0089  0.0970  0.2431  0.0676
                                    -0.1018 -0.1824  0.2274 -0.0038
596. (0.00029) RY*( 7) C  27        s(  1.63%)p11.44( 18.70%)d48.73( 79.66%)
                                     0.0000 -0.0011 -0.0458  0.1173 -0.0221
                                     0.0013  0.1070  0.0386  0.0098 -0.2919
                                     0.1806  0.0102 -0.1931 -0.1371  0.1403
                                    -0.3553 -0.7980  0.0957 -0.0689
597. (0.00025) RY*( 8) C  27        s( 17.52%)p 1.79( 31.34%)d 2.92( 51.14%)
                                     0.0000  0.0014 -0.2452  0.3379  0.0298
                                     0.0109 -0.0481 -0.1893 -0.0024 -0.0517
                                    -0.0641  0.0079 -0.0823  0.5114 -0.2067
                                    -0.4333  0.2115  0.4320 -0.2226
598. (0.00019) RY*( 9) C  27        s(  1.95%)p30.95( 60.46%)d19.24( 37.59%)
                                     0.0000  0.0049  0.1043 -0.0842  0.0393
                                     0.0152 -0.1480  0.5900  0.0024  0.0013
                                     0.2568 -0.0019  0.0670  0.4048  0.2758
                                    -0.0914  0.0554 -0.2855 -0.4549
599. (0.00016) RY*(10) C  27        s(  8.38%)p 1.78( 14.92%)d 9.15( 76.70%)
                                     0.0000  0.0007  0.0940  0.2712  0.0378
                                    -0.0056  0.1112  0.1970 -0.0180  0.1916
                                    -0.0297  0.0046  0.0233  0.2439 -0.5949
                                    -0.1443 -0.1949 -0.4841  0.3463
600. (0.00011) RY*(11) C  27        s( 24.17%)p 1.22( 29.49%)d 1.92( 46.34%)
                                     0.0000 -0.0025 -0.2651  0.4136 -0.0171
                                    -0.0027  0.0596  0.4585  0.0126 -0.0761
                                    -0.2540  0.0152 -0.0850  0.0573  0.4284
                                     0.1222  0.0838  0.1415  0.4878
601. (0.00008) RY*(12) C  27        s( 44.22%)p 0.65( 28.75%)d 0.61( 27.03%)
602. (0.00003) RY*(13) C  27        s(  4.03%)p 3.43( 13.82%)d20.37( 82.15%)
603. (0.00000) RY*(14) C  27        s( 99.27%)p 0.00(  0.16%)d 0.01(  0.57%)
604. (0.00154) RY*( 1) C  28        s(  6.61%)p11.31( 74.81%)d 2.81( 18.57%)
                                     0.0000  0.0013 -0.1670  0.1956 -0.0047
                                    -0.0037  0.2667  0.1248 -0.0058  0.0209
                                     0.0449 -0.0130 -0.8094 -0.0595  0.0400
                                    -0.3159 -0.2781  0.0572  0.0612
605. (0.00098) RY*( 2) C  28        s(  0.99%)p73.32( 72.32%)d27.07( 26.70%)
                                     0.0000  0.0015 -0.0504  0.0855 -0.0042
                                    -0.0123 -0.5298  0.1271  0.0102  0.6408
                                     0.0149 -0.0010 -0.1072  0.0607 -0.0755
                                    -0.1115 -0.0081 -0.4963 -0.0497
606. (0.00025) RY*( 3) C  28        s( 16.37%)p 4.90( 80.26%)d 0.21(  3.37%)
                                     0.0000  0.0067 -0.2362  0.3283 -0.0095
                                    -0.0079  0.5258  0.3684 -0.0074  0.4121
                                     0.3535  0.0033  0.3092  0.0007  0.0429
                                     0.1097  0.1124  0.0625 -0.0573
607. (0.00014) RY*( 4) C  28        s(  3.48%)p20.00( 69.57%)d 7.75( 26.95%)
                                     0.0000  0.0107 -0.1193  0.1318 -0.0552
                                     0.0071 -0.4089 -0.1720 -0.0047 -0.0802
                                     0.6414 -0.0033  0.0794  0.2735  0.2617
                                    -0.0880 -0.2739  0.3371  0.0684
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608. (0.00011) RY*( 5) C  28          s( 21.91%)p 3.25( 71.31%)d 0.31(  6.78%)
                                        0.0000 -0.0132 -0.0870  0.4536  0.0751
                                        0.0026 -0.0074 -0.6613 -0.0027  0.2979
                                       -0.2050 -0.0007  0.0490 -0.3775 -0.0122
                                        0.0352  0.0243  0.2283  0.1168
609. (0.00008) RY*( 6) C  28          s( 37.88%)p 1.03( 38.94%)d 0.61( 23.19%)
610. (0.00004) RY*( 7) C  28          s( 57.02%)p 0.20( 11.32%)d 0.56( 31.65%)
611. (0.00003) RY*( 8) C  28          s( 11.49%)p 7.18( 82.45%)d 0.53(  6.06%)
612. (0.00001) RY*( 9) C  28          s( 21.84%)p 0.97( 21.29%)d 2.60( 56.87%)
613. (0.00001) RY*(10) C  28          s( 13.28%)p 1.43( 19.04%)d 5.10( 67.69%)
614. (0.00001) RY*(11) C  28          s(  0.80%)p54.81( 43.70%)d69.60( 55.50%)
615. (0.00001) RY*(12) C  28          s(  5.75%)p 2.06( 11.86%)d14.33( 82.39%)
616. (0.00000) RY*(13) C  28          s( 98.81%)p 0.01(  0.99%)d 0.00(  0.19%)
617. (0.00001) RY*(14) C  28          s(  3.77%)p 0.61(  2.32%)d24.89( 93.91%)
618. (0.00356) RY*( 1) C  29          s(  2.79%)p32.06( 89.42%)d 2.79(  7.79%)
                                        0.0000  0.0047  0.1641  0.0302  0.0041
                                       -0.0156 -0.4976  0.0491  0.0239  0.7047
                                       -0.0285 -0.0084 -0.3722  0.0854 -0.1524
                                        0.1486 -0.1678 -0.0546  0.0386
619. (0.00128) RY*( 2) C  29          s(  0.71%)p99.99( 78.58%)d29.36( 20.71%)
                                        0.0000  0.0085  0.0020  0.0834  0.0038
                                       -0.0030  0.1214 -0.0067  0.0013 -0.3440
                                       -0.0554 -0.0091 -0.7731 -0.2276  0.0822
                                        0.0652 -0.3037  0.1161 -0.3007
620. (0.00112) RY*( 3) C  29          s(  0.06%)p99.99( 85.15%)d99.99( 14.79%)
                                        0.0000  0.0016  0.0199  0.0150  0.0014
                                        0.0026 -0.7529  0.1401 -0.0009 -0.4931
                                        0.1070 -0.0004  0.0942 -0.0399  0.1657
                                        0.2244  0.0899 -0.2415 -0.0604
621. (0.00066) RY*( 4) C  29          s(  1.06%)p48.76( 51.69%)d44.57( 47.25%)
                                        0.0000  0.0002  0.1030 -0.0006 -0.0008
                                       -0.0135  0.3230  0.5447 -0.0065  0.1369
                                        0.3032  0.0021 -0.0694  0.0100  0.1016
                                        0.5354  0.3598 -0.1093 -0.1846
622. (0.00050) RY*( 5) C  29          s( 50.40%)p 0.34( 17.28%)d 0.64( 32.32%)
                                        0.0000  0.0040  0.7013  0.1101 -0.0066
                                       -0.0108  0.0771  0.0560  0.0146 -0.0781
                                       -0.1786 -0.0074  0.1701 -0.3105 -0.4046
                                       -0.1275 -0.0376 -0.2983 -0.2299
623. (0.00032) RY*( 6) C  29          s(  8.37%)p 9.07( 75.93%)d 1.88( 15.70%)
                                        0.0000 -0.0024  0.2679 -0.1052  0.0287
                                       -0.0027  0.0487  0.1830  0.0094 -0.2776
                                       -0.0690  0.0068 -0.2894  0.7468 -0.2040
                                       -0.1769  0.1261 -0.0514  0.2559
624. (0.00025) RY*( 7) C  29          s(  4.32%)p11.99( 51.79%)d10.16( 43.89%)
                                        0.0000  0.0001  0.2077 -0.0049 -0.0053
                                       -0.0013  0.0059 -0.4769  0.0037 -0.0205
                                       -0.5123  0.0003  0.0273  0.1637  0.1279
                                        0.5115  0.3013  0.2288 -0.1333
625. (0.00026) RY*( 8) C  29          s( 15.51%)p 1.18( 18.35%)d 4.26( 66.14%)
                                        0.0000 -0.0029  0.3936 -0.0107 -0.0067
                                       -0.0037  0.0291  0.0963 -0.0003  0.0450
                                        0.1331 -0.0122  0.2709  0.2830  0.5201
                                        0.0036 -0.5511  0.2255 -0.1907
626. (0.00017) RY*( 9) C  29          s(  0.20%)p99.99( 21.59%)d99.99( 78.20%)
                                        0.0000  0.0025  0.0048  0.0442 -0.0079
                                        0.0190 -0.1972  0.3767  0.0066 -0.0782
                                       -0.0690 -0.0042  0.1199 -0.0974 -0.3433
                                       -0.0348  0.0757  0.8073 -0.0743
627. (0.00014) RY*(10) C  29          s(  0.88%)p63.71( 56.02%)d49.02( 43.10%)
                                        0.0000  0.0074  0.0932 -0.0052 -0.0057
                                        0.0020  0.0009  0.4105 -0.0051  0.0673
                                       -0.5549  0.0143 -0.0869 -0.2673  0.4761
                                       -0.1988  0.1309 -0.0350  0.3827
628. (0.00010) RY*(11) C  29          s( 17.83%)p 2.21( 39.44%)d 2.40( 42.72%)
629. (0.00002) RY*(12) C  29          s( 95.59%)p 0.02(  1.82%)d 0.03(  2.59%)
630. (0.00002) RY*(13) C  29          s(  2.41%)p 5.42( 13.03%)d35.16( 84.56%)
631. (0.00000) RY*(14) C  29          s( 99.83%)p 0.00(  0.12%)d 0.00(  0.05%)
632. (0.00169) RY*( 1) C  30          s(  3.14%)p25.64( 80.53%)d 5.20( 16.33%)
                                        0.0000  0.0008 -0.1059  0.1419 -0.0064
                                       -0.0027  0.2973  0.0852  0.0136  0.8061
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                                    -0.0023  0.0048  0.2433  0.0195  0.3717
                                     0.0593 -0.0953  0.0363 -0.1057
633. (0.00101) RY*( 2) C  30       s(  2.56%)p29.66( 75.87%)d 8.43( 21.57%)
                                     0.0000  0.0009 -0.1126  0.1135 -0.0044
                                    -0.0057 -0.0932  0.1002  0.0051  0.2223
                                    -0.0517 -0.0122 -0.8280  0.0452  0.1791
                                    -0.3305  0.0489 -0.0914  0.2524
634. (0.00032) RY*( 3) C  30       s( 20.08%)p 3.92( 78.77%)d 0.06(  1.15%)
                                     0.0000  0.0055 -0.3162  0.3172 -0.0125
                                    -0.0144  0.7158  0.3822 -0.0008 -0.3353
                                     0.0188  0.0034 -0.0681 -0.1081 -0.0890
                                    -0.0051  0.0492  0.0268 -0.0199
635. (0.00017) RY*( 4) C  30       s( 10.75%)p 4.85( 52.07%)d 3.46( 37.19%)
                                     0.0000  0.0007  0.3006 -0.1305 -0.0085
                                    -0.0013  0.1450  0.2746  0.0012 -0.0626
                                    -0.1860 -0.0115  0.3083  0.5391  0.0880
                                    -0.3978  0.1299 -0.1030  0.4223
636. (0.00010) RY*( 5) C  30       s( 19.55%)p 3.56( 69.64%)d 0.55( 10.80%)
                                     0.0000 -0.0172 -0.2065  0.3816  0.0836
                                    -0.0025  0.1276 -0.6569  0.0023 -0.0814
                                     0.2521 -0.0034  0.0330  0.4212  0.0661
                                     0.0874  0.1240 -0.2345  0.1603
637. (0.00007) RY*( 6) C  30       s( 44.77%)p 0.95( 42.32%)d 0.29( 12.91%)
638. (0.00003) RY*( 7) C  30       s( 36.34%)p 0.34( 12.28%)d 1.41( 51.38%)
639. (0.00003) RY*( 8) C  30       s( 12.70%)p 4.01( 50.92%)d 2.86( 36.38%)
640. (0.00001) RY*( 9) C  30       s( 32.91%)p 0.54( 17.74%)d 1.50( 49.35%)
641. (0.00001) RY*(10) C  30       s(  0.43%)p99.99( 94.18%)d12.42(  5.39%)
642. (0.00001) RY*(11) C  30       s( 13.79%)p 1.33( 18.35%)d 4.92( 67.86%)
643. (0.00001) RY*(12) C  30       s(  0.20%)p13.39(  2.70%)d99.99( 97.10%)
644. (0.00001) RY*(13) C  30       s(  3.54%)p 1.17(  4.15%)d26.06( 92.31%)
645. (0.00000) RY*(14) C  30       s( 99.23%)p 0.01(  0.66%)d 0.00(  0.11%)
646. (0.00656) RY*( 1) C  31       s(  6.29%)p13.79( 86.69%)d 1.12(  7.02%)
                                     0.0000  0.0078  0.2402  0.0716  0.0032
                                     0.0128 -0.6562 -0.0227 -0.0077  0.2615
                                     0.0217  0.0137 -0.6047 -0.0303  0.0154
                                     0.1913 -0.1295  0.1271 -0.0218
647. (0.00339) RY*( 2) C  31       s(  0.39%)p99.99( 96.13%)d 8.82(  3.48%)
                                     0.0000 -0.0019  0.0596 -0.0196 -0.0031
                                    -0.0037 -0.6070  0.1027 -0.0029 -0.6412
                                    -0.0270 -0.0002  0.4121  0.0240 -0.0685
                                     0.0424 -0.1163 -0.0855  0.0864
648. (0.00263) RY*( 3) C  31       s(  0.05%)p99.99( 87.83%)d99.99( 12.12%)
                                     0.0000  0.0020  0.0230 -0.0034  0.0009
                                    -0.0047  0.2919  0.0019  0.0081 -0.6578
                                     0.0237  0.0051 -0.5984  0.0404 -0.1972
                                    -0.0846 -0.0964 -0.0130 -0.2562
649. (0.00107) RY*( 4) C  31       s( 42.97%)p 1.19( 51.30%)d 0.13(  5.73%)
                                     0.0000 -0.0045  0.6545  0.0365 -0.0046
                                     0.0003  0.0677 -0.5544 -0.0048 -0.0515
                                     0.0915  0.0067  0.1182 -0.4195 -0.0037
                                    -0.1283  0.1099 -0.1590 -0.0586
650. (0.00083) RY*( 5) C  31       s(  4.50%)p 1.42(  6.39%)d19.82( 89.11%)
                                     0.0000 -0.0006  0.1594 -0.1398  0.0027
                                    -0.0078 -0.0006 -0.0738 -0.0077 -0.0040
                                     0.1276  0.0047  0.0185  0.2042 -0.1803
                                    -0.5435 -0.1456  0.6384  0.3667
651. (0.00075) RY*( 6) C  31       s( 72.07%)p 0.20( 14.69%)d 0.18( 13.24%)
                                     0.0000  0.0012 -0.3389  0.7783 -0.0012
                                     0.0061 -0.0498 -0.1070  0.0037  0.0145
                                     0.0218  0.0074  0.0650 -0.3578 -0.1815
                                    -0.1621 -0.2003  0.1627 -0.0811
652. (0.00059) RY*( 7) C  31       s( 10.98%)p 4.68( 51.34%)d 3.43( 37.68%)
                                     0.0000 -0.0001 -0.1188  0.3093 -0.0013
                                     0.0049  0.0246 -0.4102 -0.0097 -0.1908
                                     0.3694 -0.0045 -0.0891  0.4045  0.4260
                                     0.2093  0.2021  0.0017  0.3327
653. (0.00044) RY*( 8) C  31       s(  0.83%)p82.57( 68.40%)d37.14( 30.77%)
                                     0.0000 -0.0005  0.0039  0.0908  0.0051
                                    -0.0085 -0.0998 -0.3466 -0.0030  0.0011
                                    -0.6216  0.0073  0.0928  0.3986  0.1442
                                    -0.1149  0.1267  0.2099 -0.4622
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654. (0.00035) RY*( 9) C  31          s(  8.93%)p 5.73( 51.19%)d 4.46( 39.88%)
                                        0.0000  0.0011  0.2181  0.2044  0.0039
                                        0.0019  0.1372  0.3372 -0.0095 -0.1687
                                       -0.5078 -0.0042 -0.1267 -0.2772  0.4195
                                        0.0210  0.1572  0.1550  0.4167
655. (0.00029) RY*(10) C  31          s( 46.95%)p 0.97( 45.44%)d 0.16(  7.60%)
                                        0.0000  0.0027  0.5224  0.4433  0.0063
                                       -0.0014  0.1062  0.4472  0.0030  0.0964
                                        0.1843  0.0011  0.1191  0.4309 -0.0150
                                       -0.0919 -0.0868 -0.1506 -0.1928
656. (0.00012) RY*(11) C  31          s(  0.85%)p30.23( 25.65%)d86.61( 73.50%)
                                        0.0000  0.0006  0.0841  0.0374  0.0020
                                        0.0090  0.1813 -0.2479  0.0006  0.0638
                                       -0.3428  0.0032  0.0090  0.2013 -0.2247
                                        0.2621 -0.6500 -0.2378  0.3698
657. (0.00013) RY*(12) C  31          s(  2.66%)p 4.15( 11.03%)d32.47( 86.31%)
                                        0.0000 -0.0076  0.1580 -0.0309  0.0249
                                        0.0157  0.1866  0.0293 -0.0055 -0.0803
                                        0.1322  0.0156  0.1998 -0.1013 -0.0246
                                        0.6562 -0.1206  0.6075 -0.2199
658. (0.00005) RY*(13) C  31          s(  2.93%)p 1.37(  4.02%)d31.79( 93.05%)
659. (0.00000) RY*(14) C  31          s( 99.64%)p 0.00(  0.03%)d 0.00(  0.33%)
660. (0.00502) RY*( 1) C  32          s(  0.62%)p99.99( 92.33%)d11.33(  7.05%)
                                        0.0000  0.0014  0.0108  0.0781 -0.0019
                                        0.0130 -0.4209  0.0333 -0.0189  0.7145
                                       -0.0220 -0.0097  0.4830 -0.0118 -0.1535
                                       -0.0697 -0.0732  0.0647 -0.1804
661. (0.00294) RY*( 2) C  32          s(  2.28%)p38.97( 88.97%)d 3.83(  8.74%)
                                        0.0000  0.0009  0.1488 -0.0261  0.0019
                                        0.0002 -0.1167 -0.0031 -0.0034  0.4803
                                        0.0580 -0.0033 -0.8004 -0.0373  0.0177
                                       -0.2386  0.1396  0.0747  0.0718
662. (0.00278) RY*( 3) C  32          s(  4.86%)p17.97( 87.36%)d 1.60(  7.78%)
                                        0.0000 -0.0012  0.2200  0.0130  0.0059
                                       -0.0015 -0.8208 -0.0872 -0.0041 -0.4197
                                       -0.0554 -0.0024 -0.0992  0.0562 -0.0443
                                       -0.0552  0.0731 -0.2509 -0.0670
663. (0.00147) RY*( 4) C  32          s( 88.84%)p 0.10(  8.63%)d 0.03(  2.52%)
                                        0.0000 -0.0025  0.9398 -0.0720 -0.0048
                                       -0.0142  0.1847 -0.1409  0.0016  0.0180
                                        0.0568  0.0049  0.1575 -0.0616  0.0718
                                        0.0817  0.0040  0.1156  0.0040
664. (0.00065) RY*( 5) C  32          s(  1.75%)p 6.46( 11.34%)d49.54( 86.91%)
                                        0.0000 -0.0023  0.1074  0.0773  0.0046
                                        0.0012  0.0066  0.1462  0.0045 -0.0230
                                       -0.2504 -0.0041  0.0113  0.1691 -0.3973
                                       -0.2552 -0.4924 -0.0334  0.6345
665. (0.00051) RY*( 6) C  32          s(  7.69%)p 9.32( 71.63%)d 2.69( 20.68%)
                                        0.0000 -0.0065  0.1376  0.2405  0.0090
                                       -0.0111 -0.0039  0.6445  0.0024  0.0078
                                        0.0495 -0.0130 -0.1464  0.5260 -0.0011
                                        0.3651 -0.1012  0.0312 -0.2497
666. (0.00049) RY*( 7) C  32          s( 54.50%)p 0.63( 34.47%)d 0.20( 11.03%)
                                        0.0000  0.0043  0.0865  0.7332  0.0013
                                        0.0060  0.1296  0.1231  0.0050 -0.0139
                                       -0.3229  0.0001 -0.0357 -0.4549  0.0283
                                       -0.1052  0.0490 -0.2761 -0.1409
667. (0.00028) RY*( 8) C  32          s( 28.96%)p 2.14( 61.96%)d 0.31(  9.07%)
                                        0.0000 -0.0008 -0.0206  0.5375 -0.0172
                                       -0.0052  0.0520 -0.3426  0.0020 -0.0320
                                        0.5768  0.0061  0.0820  0.3988 -0.0289
                                       -0.2474  0.1245  0.0066  0.1147
668. (0.00021) RY*( 9) C  32          s(  4.28%)p 3.13( 13.39%)d19.25( 82.34%)
                                        0.0000  0.0001 -0.0418  0.2025  0.0022
                                       -0.0125 -0.2068  0.1483 -0.0102 -0.1967
                                       -0.0718  0.0019  0.0358 -0.1540  0.2235
                                       -0.1349  0.0134  0.8635  0.0969
669. (0.00015) RY*(10) C  32          s(  1.98%)p18.74( 37.14%)d30.72( 60.88%)
                                        0.0000  0.0027 -0.0459  0.1331  0.0013
                                       -0.0067  0.0205 -0.5309 -0.0003 -0.0279
                                       -0.1698 -0.0162 -0.2338  0.0669 -0.2545
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                                      0.2601 -0.5104  0.2239 -0.4072
670. (0.00012) RY*(11) C  32          s(  3.93%)p 2.92( 11.47%)d21.53( 84.60%)
                                      0.0000 -0.0014 -0.0606  0.1883 -0.0120
                                     -0.0061 -0.1689 -0.2121  0.0110  0.1903
                                     -0.0579  0.0015 -0.0297 -0.0234  0.3787
                                      0.6554 -0.0104 -0.0691  0.5179
671. (0.00007) RY*(12) C  32          s(  0.02%)p99.99( 74.86%)d99.99( 25.13%)
672. (0.00004) RY*(13) C  32          s(  1.42%)p 4.50(  6.41%)d64.77( 92.17%)
673. (0.00000) RY*(14) C  32          s( 98.88%)p 0.00(  0.19%)d 0.01(  0.93%)
674. (0.00405) RY*( 1) C  33          s(  1.68%)p53.09( 89.26%)d 5.39(  9.06%)
                                      0.0000  0.0055  0.1284 -0.0168  0.0035
                                     -0.0007 -0.0682 -0.1148 -0.0134 -0.4689
                                      0.0462 -0.0211 -0.8061 -0.0488  0.1574
                                     -0.0105  0.1414 -0.0957  0.1912
675. (0.00148) RY*( 2) C  33          s(  0.51%)p99.99( 95.52%)d 7.82(  3.97%)
                                      0.0000  0.0052  0.0698  0.0121  0.0057
                                      0.0212 -0.4082 -0.1524 -0.0103  0.7641
                                     -0.1432  0.0048 -0.4001  0.0198 -0.1404
                                     -0.0479 -0.0740 -0.0880  0.0670
676. (0.00134) RY*( 3) C  33          s(  0.07%)p99.99( 92.95%)d99.99(  6.98%)
                                      0.0000 -0.0045 -0.0168  0.0177 -0.0076
                                     -0.0115  0.8614 -0.1184  0.0106  0.2320
                                     -0.2176 -0.0063 -0.2055  0.1726 -0.0720
                                      0.0182 -0.1557 -0.0950  0.1761
677. (0.00059) RY*( 4) C  33          s( 94.05%)p 0.04(  3.29%)d 0.03(  2.66%)
                                      0.0000 -0.0009  0.9606 -0.1328 -0.0046
                                     -0.0117  0.0654 -0.0649  0.0163  0.0160
                                      0.0662  0.0129  0.1298  0.0490  0.0061
                                     -0.1385 -0.0127  0.0123 -0.0841
678. (0.00046) RY*( 5) C  33          s(  0.48%)p19.90(  9.47%)d99.99( 90.05%)
                                      0.0000 -0.0002  0.0581  0.0366  0.0066
                                     -0.0055 -0.1384 -0.0452 -0.0041 -0.2018
                                     -0.1198  0.0032  0.1347  0.0159 -0.2763
                                      0.2828 -0.3065 -0.8041  0.0609
679. (0.00015) RY*( 6) C  33          s(  1.86%)p16.91( 31.50%)d35.76( 66.64%)
                                      0.0000 -0.0049  0.1261  0.0491 -0.0175
                                      0.0172 -0.0747  0.3984 -0.0072  0.1110
                                      0.1124  0.0108 -0.0201  0.3534  0.3618
                                      0.6398 -0.1421  0.1378  0.2949
680. (0.00009) RY*( 7) C  33          s(  9.31%)p 6.82( 63.52%)d 2.92( 27.17%)
681. (0.00008) RY*( 8) C  33          s(  3.11%)p22.94( 71.33%)d 8.22( 25.56%)
682. (0.00005) RY*( 9) C  33          s(  9.98%)p 2.09( 20.86%)d 6.93( 69.16%)
683. (0.00004) RY*(10) C  33          s(  6.54%)p12.60( 82.36%)d 1.70( 11.10%)
684. (0.00003) RY*(11) C  33          s( 20.44%)p 0.27(  5.55%)d 3.62( 74.02%)
685. (0.00002) RY*(12) C  33          s( 54.08%)p 0.35( 18.92%)d 0.50( 27.00%)
686. (0.00001) RY*(13) C  33          s(  0.96%)p16.17( 15.53%)d86.99( 83.51%)
687. (0.00000) RY*(14) C  33          s( 96.98%)p 0.00(  0.07%)d 0.03(  2.94%)
688. (0.00413) RY*( 1) C  34          s(  0.96%)p94.35( 91.02%)d 8.31(  8.02%)
                                      0.0000  0.0011  0.0904  0.0380  0.0061
                                     -0.0242 -0.7342  0.0528  0.0072  0.1953
                                     -0.0111 -0.0199 -0.5719  0.0439  0.0297
                                      0.1888 -0.1667  0.1242 -0.0206
689. (0.00186) RY*( 2) C  34          s(  0.02%)p99.99( 99.98%)d 0.34(  0.01%)
                                      0.0000  0.0001 -0.0084  0.0097 -0.0005
                                     -0.0133  0.3022  0.1094  0.0269 -0.6581
                                     -0.2076  0.0251 -0.6140 -0.2042  0.0022
                                      0.0003  0.0020  0.0066  0.0018
690. (0.00087) RY*( 3) C  34          s(  0.03%)p99.99( 90.29%)d99.99(  9.68%)
                                      0.0000  0.0021 -0.0107  0.0151  0.0000
                                     -0.0017 -0.5083  0.1148 -0.0036 -0.6400
                                      0.1537  0.0016  0.4356 -0.0909  0.1402
                                      0.0732  0.1529  0.0316 -0.2177
691. (0.00054) RY*( 4) C  34          s( 88.32%)p 0.02(  1.50%)d 0.12( 10.18%)
                                      0.0000 -0.0011  0.9347  0.0975  0.0060
                                      0.0109  0.0221 -0.0595 -0.0062 -0.0648
                                     -0.0082  0.0116  0.0738 -0.0307 -0.0379
                                     -0.1876 -0.0142  0.2025  0.1548
692. (0.00052) RY*( 5) C  34          s( 11.14%)p 0.37(  4.17%)d 7.60( 84.68%)
                                      0.0000 -0.0006  0.3087  0.1269  0.0023
                                      0.0093  0.1144  0.0601  0.0047  0.1208
                                      0.0245 -0.0014 -0.0523 -0.0836  0.0863
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                                      0.4700  0.1323 -0.6408 -0.4364
693. (0.00019) RY*( 6) C  34          s(  0.01%)p99.99( 28.53%)d99.99( 71.45%)
                                      0.0000 -0.0003  0.0106  0.0049  0.0003
                                     -0.0106  0.0535 -0.1714  0.0222 -0.1107
                                      0.3392  0.0215 -0.1070  0.3365  0.4997
                                      0.2631  0.2512 -0.1161  0.5648
694. (0.00007) RY*( 7) C  34          s( 39.08%)p 0.78( 30.38%)d 0.78( 30.54%)
695. (0.00005) RY*( 8) C  34          s( 12.97%)p 5.96( 77.33%)d 0.75(  9.70%)
696. (0.00003) RY*( 9) C  34          s(  6.97%)p 8.85( 61.68%)d 4.50( 31.35%)
697. (0.00003) RY*(10) C  34          s(  4.70%)p 4.29( 20.17%)d15.99( 75.13%)
698. (0.00003) RY*(11) C  34          s( 31.71%)p 1.85( 58.69%)d 0.30(  9.59%)
699. (0.00000) RY*(12) C  34          s( 98.70%)p 0.00(  0.37%)d 0.01(  0.93%)
700. (0.00000) RY*(13) C  34          s(  5.36%)p 4.00( 21.44%)d13.67( 73.20%)
701. (0.00001) RY*(14) C  34          s(  0.06%)p99.99( 14.60%)d99.99( 85.34%)
702. (0.00425) RY*( 1) C  35          s(  1.84%)p48.64( 89.43%)d 4.75(  8.73%)
                                      0.0000  0.0058  0.1337 -0.0216  0.0035
                                     -0.0152 -0.6070 -0.0703  0.0182  0.6636
                                     -0.0198  0.0085  0.2619 -0.1049 -0.1598
                                     -0.1713 -0.0072 -0.0314 -0.1771
703. (0.00143) RY*( 2) C  35          s(  0.37%)p99.99( 98.30%)d 3.61(  1.34%)
                                      0.0000  0.0067  0.0599  0.0019  0.0079
                                      0.0164 -0.4563 -0.0972  0.0047 -0.0732
                                      0.0033  0.0232 -0.8712  0.0110  0.0029
                                      0.0036  0.0489 -0.0647  0.0822
704. (0.00118) RY*( 3) C  35          s(  0.31%)p99.99( 93.27%)d20.50(  6.42%)
                                      0.0000  0.0041  0.0428 -0.0359 -0.0009
                                     -0.0040 -0.5557  0.1630 -0.0071 -0.6466
                                      0.2307  0.0058  0.3172 -0.1591  0.0867
                                     -0.1019  0.0912  0.1931 -0.0267
705. (0.00061) RY*( 4) C  35          s( 92.57%)p 0.04(  3.98%)d 0.04(  3.45%)
                                      0.0000 -0.0018  0.9568 -0.1009 -0.0055
                                      0.0051  0.1454  0.0569 -0.0141 -0.0505
                                     -0.0429 -0.0184  0.0032 -0.1024  0.0275
                                     -0.0672 -0.0311 -0.0805  0.1476
706. (0.00048) RY*( 5) C  35          s(  1.55%)p 1.50(  2.33%)d61.84( 96.12%)
                                      0.0000  0.0009  0.1136 -0.0500 -0.0117
                                     -0.0028  0.0787 -0.0067 -0.0063  0.0757
                                      0.0204  0.0026 -0.0814 -0.0651  0.4550
                                      0.2482  0.4855  0.1116 -0.6666
707. (0.00015) RY*( 6) C  35          s(  1.01%)p34.68( 35.09%)d63.17( 63.90%)
                                      0.0000 -0.0051  0.0934  0.0343 -0.0141
                                      0.0126 -0.0204  0.5418 -0.0016 -0.0136
                                     -0.0666  0.0166 -0.1261  0.1895 -0.3319
                                      0.2575 -0.4495  0.3073 -0.4075
708. (0.00009) RY*( 7) C  35          s(  0.83%)p99.99( 92.98%)d 7.49(  6.19%)
709. (0.00009) RY*( 8) C  35          s(  0.73%)p87.03( 63.72%)d48.55( 35.55%)
710. (0.00007) RY*( 9) C  35          s(  5.32%)p 7.44( 39.56%)d10.36( 55.12%)
711. (0.00004) RY*(10) C  35          s( 37.44%)p 0.50( 18.83%)d 1.17( 43.73%)
712. (0.00002) RY*(11) C  35          s(  1.70%)p11.25( 19.14%)d46.54( 79.16%)
713. (0.00002) RY*(12) C  35          s(  0.91%)p25.87( 23.60%)d82.77( 75.49%)
714. (0.00002) RY*(13) C  35          s( 57.28%)p 0.35( 19.87%)d 0.40( 22.85%)
715. (0.00000) RY*(14) C  35          s( 98.15%)p 0.00(  0.05%)d 0.02(  1.79%)
716. (0.00522) RY*( 1) C  36          s(  0.63%)p99.99( 92.52%)d10.92(  6.85%)
                                      0.0000  0.0013  0.0026  0.0791 -0.0026
                                     -0.0028  0.1936  0.0078  0.0138 -0.6125
                                      0.0148  0.0219 -0.7149  0.0236  0.1494
                                      0.1061  0.0612 -0.0227  0.1753
717. (0.00289) RY*( 2) C  36          s(  3.29%)p26.45( 87.09%)d 2.92(  9.62%)
                                      0.0000 -0.0010  0.1813  0.0062  0.0054
                                     -0.0023 -0.8835 -0.0413  0.0041  0.0552
                                     -0.0290  0.0031 -0.2910 -0.0099 -0.0147
                                     -0.2534  0.1483 -0.0399  0.0901
718. (0.00273) RY*( 3) C  36          s(  1.32%)p67.71( 89.27%)d 7.14(  9.41%)
                                      0.0000  0.0025  0.1139  0.0141  0.0021
                                      0.0005  0.2378  0.0492  0.0057  0.7233
                                      0.0870 -0.0015 -0.5497 -0.0291  0.1010
                                      0.0630  0.1480 -0.1522 -0.1867
719. (0.00147) RY*( 4) C  36          s( 89.23%)p 0.08(  7.02%)d 0.04(  3.75%)
                                      0.0000 -0.0027  0.9417 -0.0735 -0.0045
                                     -0.0056  0.1424 -0.1158 -0.0070 -0.0998
                                      0.0456 -0.0085  0.1040 -0.1161  0.0233
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                                    0.0125  0.0163  0.1836 -0.0535
720. (0.00078) RY*( 5) C  36        s(  8.07%)p 3.95( 31.90%)d 7.44( 60.03%)
                                    0.0000 -0.0050  0.2398  0.1521  0.0060
                                   -0.0160 -0.0882  0.4448 -0.0086 -0.0305
                                   -0.2210  0.0009  0.0411  0.2482 -0.2015
                                    0.3273 -0.2885 -0.6058  0.0481
721. (0.00050) RY*( 6) C  36        s( 42.21%)p 0.96( 40.50%)d 0.41( 17.29%)
                                    0.0000  0.0053  0.0411  0.6484  0.0001
                                    0.0080  0.0551 -0.4053 -0.0059 -0.0393
                                    0.4550  0.0037  0.1158  0.1247  0.0087
                                   -0.2014  0.0380 -0.3617 -0.0020
722. (0.00044) RY*( 7) C  36        s( 21.45%)p 1.51( 32.34%)d 2.15( 46.21%)
                                    0.0000 -0.0015  0.0580  0.4595  0.0036
                                   -0.0006  0.0367  0.4198  0.0150  0.1714
                                    0.0201 -0.0123 -0.0172  0.3397  0.0744
                                   -0.1398 -0.1214  0.5483  0.3488
723. (0.00027) RY*( 8) C  36        s( 21.70%)p 3.18( 69.03%)d 0.43(  9.27%)
                                    0.0000 -0.0006 -0.0157  0.4652 -0.0207
                                    0.0009  0.0687  0.2200 -0.0060 -0.0462
                                   -0.4461 -0.0034  0.0541 -0.6581  0.0144
                                   -0.1699  0.2243 -0.0505 -0.1035
724. (0.00020) RY*( 9) C  36        s(  4.74%)p 2.15( 10.21%)d17.93( 85.05%)
                                    0.0000 -0.0001 -0.0315  0.2154 -0.0042
                                   -0.0163 -0.2482  0.0626 -0.0028 -0.0806
                                    0.0688  0.0027  0.1166  0.1071  0.5037
                                    0.5629  0.1877  0.1650 -0.4663
725. (0.00011) RY*(10) C  36        s(  5.40%)p 4.60( 24.83%)d12.92( 69.77%)
                                    0.0000 -0.0007 -0.0513  0.2267 -0.0005
                                   -0.0073 -0.1392 -0.3080  0.0022  0.0844
                                    0.0157 -0.0125 -0.1958 -0.2969 -0.3975
                                    0.3904 -0.5490  0.2853 -0.0664
726. (0.00012) RY*(11) C  36        s(  0.12%)p99.99( 16.70%)d99.99( 83.18%)
                                    0.0000 -0.0027 -0.0092  0.0311 -0.0128
                                    0.0083  0.0362  0.2257 -0.0110 -0.1927
                                    0.0726 -0.0021 -0.1299  0.2350 -0.4245
                                   -0.3341 -0.0011  0.1390 -0.7216
727. (0.00007) RY*(12) C  36        s(  1.40%)p68.52( 96.02%)d 1.84(  2.58%)
728. (0.00004) RY*(13) C  36        s(  1.18%)p 2.14(  2.52%)d81.57( 96.30%)
729. (0.00000) RY*(14) C  36        s( 99.28%)p 0.00(  0.21%)d 0.01(  0.51%)
730. (0.00347) RY*( 1) C  37        s(  2.63%)p34.07( 89.62%)d 2.95(  7.75%)
                                    0.0000  0.0040  0.1587  0.0329  0.0037
                                    0.0170  0.6112 -0.0787  0.0061  0.1011
                                    0.0516  0.0225  0.7080 -0.0385 -0.0335
                                    0.2408  0.0107  0.1334 -0.0210
731. (0.00128) RY*( 2) C  37        s(  0.93%)p83.10( 77.43%)d23.23( 21.64%)
                                    0.0000  0.0081  0.0093  0.0957  0.0031
                                    0.0090  0.5572  0.1102 -0.0034 -0.4651
                                   -0.2228  0.0014 -0.4308 -0.0088  0.2844
                                    0.0825 -0.2720  0.1680  0.1629
732. (0.00115) RY*( 3) C  37        s(  0.73%)p99.99( 86.33%)d17.78( 12.94%)
                                    0.0000 -0.0025  0.0805 -0.0282 -0.0017
                                    0.0005  0.3151 -0.1490  0.0007  0.7558
                                   -0.0763  0.0058 -0.4003  0.0659 -0.1109
                                   -0.1212  0.0903  0.1994  0.2336
733. (0.00063) RY*( 4) C  37        s(  0.70%)p68.19( 47.40%)d74.67( 51.90%)
                                    0.0000  0.0026  0.0780  0.0294 -0.0006
                                   -0.0050  0.1840  0.1705 -0.0097  0.1269
                                    0.4063  0.0072 -0.2503 -0.4087 -0.0962
                                    0.3785 -0.0747 -0.5972 -0.0650
734. (0.00052) RY*( 5) C  37        s( 42.68%)p 0.56( 23.81%)d 0.79( 33.51%)
                                    0.0000  0.0042  0.6390  0.1354 -0.0081
                                    0.0135 -0.2173  0.3426  0.0007  0.0516
                                   -0.2411  0.0141 -0.0040 -0.1112  0.3064
                                    0.2361  0.4027  0.0816  0.1291
735. (0.00034) RY*( 6) C  37        s( 18.83%)p 3.73( 70.24%)d 0.58( 10.93%)
                                    0.0000 -0.0009  0.4290 -0.0624  0.0200
                                    0.0013  0.0065 -0.7085  0.0107 -0.3372
                                    0.1529  0.0073 -0.1429 -0.2065 -0.2258
                                   -0.0818  0.2108  0.0359  0.0768
736. (0.00026) RY*( 7) C  37        s( 15.39%)p 1.08( 16.62%)d 4.42( 68.00%)
                                    0.0000 -0.0012  0.3917 -0.0164 -0.0147
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                                     0.0091 -0.2178 -0.2423 -0.0074  0.2150
                                    -0.0837  0.0005  0.0729  0.0363  0.2658
                                     0.0345 -0.7694 -0.0654 -0.1087
737. (0.00024) RY*( 8) C  37        s(  0.58%)p99.99( 62.41%)d63.36( 37.00%)
                                     0.0000 -0.0019  0.0750  0.0142  0.0032
                                     0.0056 -0.0638  0.2303 -0.0010 -0.0056
                                     0.7282 -0.0028 -0.0070 -0.1914  0.1852
                                    -0.2265 -0.1083  0.5162  0.0788
738. (0.00017) RY*( 9) C  37        s(  0.84%)p13.12( 10.96%)d99.99( 88.20%)
                                     0.0000  0.0016 -0.0538  0.0703 -0.0227
                                     0.0109 -0.1803  0.1050  0.0107 -0.0644
                                    -0.0869 -0.0142  0.1676 -0.1609 -0.3622
                                     0.0838 -0.2479 -0.0100  0.8260
739. (0.00014) RY*(10) C  37        s(  0.95%)p80.29( 76.12%)d24.19( 22.94%)
                                     0.0000 -0.0081  0.0812 -0.0510  0.0150
                                     0.0109 -0.0445 -0.0660 -0.0021 -0.0686
                                     0.3609  0.0088 -0.0956  0.7814  0.0090
                                     0.4374  0.0448 -0.0382  0.1856
740. (0.00011) RY*(11) C  37        s( 20.31%)p 1.22( 24.71%)d 2.71( 54.98%)
                                     0.0000  0.0012  0.4130 -0.1785 -0.0260
                                    -0.0059  0.1091  0.4193  0.0161 -0.1145
                                    -0.0500  0.0120 -0.0704  0.1958 -0.6357
                                    -0.2206 -0.1699  0.0473 -0.2566
741. (0.00002) RY*(12) C  37        s(  3.08%)p 4.12( 12.67%)d27.40( 84.25%)
742. (0.00002) RY*(13) C  37        s( 92.52%)p 0.02(  1.80%)d 0.06(  5.68%)
743. (0.00000) RY*(14) C  37        s( 99.79%)p 0.00(  0.11%)d 0.00(  0.10%)
744. (0.00174) RY*( 1) C  38        s(  2.32%)p35.38( 81.96%)d 6.79( 15.72%)
                                     0.0000  0.0006 -0.0782  0.1304 -0.0062
                                     0.0020  0.1880 -0.0155  0.0123  0.8765
                                     0.0396  0.0078  0.0947 -0.0715  0.1783
                                    -0.0643 -0.2895 -0.0833 -0.1747
745. (0.00102) RY*( 2) C  38        s(  2.67%)p28.76( 76.80%)d 7.69( 20.53%)
                                     0.0000  0.0011 -0.1107  0.1201 -0.0047
                                     0.0125  0.8320 -0.0463 -0.0037 -0.2425
                                     0.0053  0.0056  0.0601 -0.1051 -0.0019
                                    -0.3784  0.1172  0.0901 -0.2006
746. (0.00031) RY*( 3) C  38        s( 17.51%)p 4.63( 81.08%)d 0.08(  1.41%)
                                     0.0000  0.0064 -0.2669  0.3218 -0.0171
                                    -0.0048 -0.0197  0.1964 -0.0041  0.0161
                                     0.1017  0.0131 -0.7853 -0.3799 -0.0107
                                     0.0282  0.0247 -0.0312  0.1079
747. (0.00018) RY*( 4) C  38        s( 12.62%)p 3.98( 50.29%)d 2.94( 37.08%)
                                     0.0000  0.0038  0.3239 -0.1437 -0.0252
                                     0.0101 -0.2725 -0.4667 -0.0046  0.1379
                                     0.2076  0.0001 -0.1041 -0.3712 -0.1601
                                    -0.4781  0.2581  0.1572 -0.1590
748. (0.00009) RY*( 5) C  38        s( 23.57%)p 2.67( 62.82%)d 0.58( 13.61%)
749. (0.00007) RY*( 6) C  38        s( 46.97%)p 0.89( 41.63%)d 0.24( 11.41%)
750. (0.00003) RY*( 7) C  38        s( 26.15%)p 1.96( 51.32%)d 0.86( 22.53%)
751. (0.00003) RY*( 8) C  38        s(  8.56%)p 2.19( 18.78%)d 8.49( 72.66%)
752. (0.00001) RY*( 9) C  38        s( 47.39%)p 0.54( 25.45%)d 0.57( 27.15%)
753. (0.00000) RY*(10) C  38        s(  0.91%)p 2.82(  2.56%)d99.99( 96.54%)
754. (0.00001) RY*(11) C  38        s(  0.38%)p99.99( 99.10%)d 1.36(  0.52%)
755. (0.00000) RY*(12) C  38        s( 99.19%)p 0.01(  0.73%)d 0.00(  0.08%)
756. (0.00001) RY*(13) C  38        s(  2.69%)p 0.51(  1.37%)d35.65( 95.94%)
757. (0.00001) RY*(14) C  38        s(  9.07%)p 0.69(  6.30%)d 9.33( 84.63%)
758. (0.00358) RY*( 1) C  39        s(  3.11%)p28.66( 89.23%)d 2.46(  7.66%)
                                     0.0000  0.0041  0.1727  0.0357  0.0050
                                     0.0250  0.7755 -0.0500 -0.0165 -0.4090
                                    -0.0042  0.0085  0.3344 -0.0908 -0.1242
                                     0.2149 -0.0570  0.1080  0.0092
759. (0.00126) RY*( 2) C  39        s(  0.74%)p99.99( 78.35%)d28.15( 20.91%)
                                     0.0000  0.0076  0.0056  0.0856  0.0024
                                     0.0037  0.1499 -0.0257 -0.0006  0.6808
                                     0.0997  0.0082  0.4664  0.2634  0.1062
                                     0.0734 -0.3740  0.0306 -0.2272
760. (0.00115) RY*( 3) C  39        s(  1.08%)p76.42( 82.17%)d15.58( 16.75%)
                                     0.0000  0.0055  0.0903  0.0507  0.0022
                                     0.0023 -0.5006  0.1274  0.0013 -0.3630
                                     0.1470  0.0025  0.6335 -0.0132 -0.0857
                                    -0.1726 -0.1427  0.3094  0.1194
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761. (0.00064) RY*( 4) C  39          s(  1.01%)p52.66( 53.38%)d44.99( 45.60%)
                                        0.0000 -0.0007  0.0956 -0.0314 -0.0013
                                       -0.0072  0.1818  0.2807 -0.0106  0.3144
                                        0.3356  0.0035 -0.1229 -0.4418 -0.2582
                                       -0.3101 -0.1883  0.0728  0.5025
762. (0.00052) RY*( 5) C  39          s( 47.39%)p 0.48( 22.72%)d 0.63( 29.90%)
                                        0.0000  0.0044  0.6777  0.1208 -0.0086
                                        0.0133 -0.0776  0.0128 -0.0100  0.0140
                                        0.2715  0.0087 -0.2486  0.2914 -0.4361
                                       -0.0069  0.0698  0.0877 -0.3102
763. (0.00031) RY*( 6) C  39          s(  5.44%)p11.81( 64.24%)d 5.57( 30.32%)
                                        0.0000 -0.0024  0.2155 -0.0842  0.0296
                                        0.0080 -0.1545 -0.4522 -0.0074  0.2407
                                       -0.1800 -0.0085  0.3309 -0.4626 -0.2852
                                        0.1129  0.3455 -0.2996  0.0022
764. (0.00026) RY*( 7) C  39          s( 22.14%)p 1.38( 30.64%)d 2.13( 47.22%)
                                        0.0000 -0.0039  0.4689 -0.0390 -0.0020
                                        0.0065 -0.0859 -0.3402  0.0004 -0.0630
                                       -0.3100  0.0099 -0.1984 -0.2089  0.3802
                                       -0.0434 -0.5474  0.1360  0.0875
765. (0.00021) RY*( 8) C  39          s(  3.17%)p13.14( 41.64%)d17.42( 55.19%)
                                        0.0000 -0.0005  0.1652 -0.0661  0.0056
                                       -0.0004 -0.0257  0.3309 -0.0025  0.0636
                                        0.2718  0.0024  0.0103 -0.4778  0.4734
                                        0.2081  0.2621  0.2157 -0.4114
766. (0.00017) RY*( 9) C  39          s(  0.10%)p99.99( 51.45%)d99.99( 48.45%)
                                        0.0000 -0.0063 -0.0075  0.0264  0.0141
                                       -0.0031  0.0573  0.2114 -0.0159  0.2249
                                       -0.6441  0.0111 -0.0211 -0.0164 -0.2111
                                       -0.0919  0.2123  0.6202 -0.0416
767. (0.00014) RY*(10) C  39          s(  0.63%)p69.51( 43.74%)d88.39( 55.63%)
                                        0.0000 -0.0052 -0.0294  0.0734 -0.0032
                                        0.0119 -0.1283  0.5114  0.0106 -0.0960
                                       -0.3138  0.0058 -0.0131 -0.2266 -0.2999
                                        0.2572 -0.4171 -0.4015 -0.2549
768. (0.00010) RY*(11) C  39          s( 18.27%)p 1.63( 29.81%)d 2.84( 51.92%)
769. (0.00002) RY*(12) C  39          s(  2.32%)p 4.84( 11.23%)d37.27( 86.45%)
770. (0.00002) RY*(13) C  39          s( 94.74%)p 0.02(  1.50%)d 0.04(  3.76%)
771. (0.00000) RY*(14) C  39          s( 99.81%)p 0.00(  0.12%)d 0.00(  0.07%)
772. (0.00162) RY*( 1) C  40          s(  3.58%)p22.18( 79.28%)d 4.80( 17.15%)
                                        0.0000  0.0007 -0.1167  0.1486 -0.0066
                                        0.0105  0.6975  0.0141 -0.0081 -0.0529
                                        0.0721 -0.0062 -0.5408 -0.0730  0.2889
                                       -0.1669 -0.1781  0.1622  0.0463
773. (0.00097) RY*( 2) C  40          s(  2.89%)p25.21( 72.76%)d 8.44( 24.36%)
                                        0.0000  0.0012 -0.1157  0.1244 -0.0037
                                        0.0080  0.4559 -0.0588 -0.0011  0.2545
                                        0.0970  0.0129  0.6593 -0.0843  0.2826
                                       -0.0305  0.3966 -0.0329 -0.0662
774. (0.00029) RY*( 3) C  40          s( 20.74%)p 3.68( 76.31%)d 0.14(  2.96%)
                                        0.0000  0.0067 -0.3215  0.3221 -0.0155
                                       -0.0044 -0.2136  0.1433 -0.0129  0.6768
                                        0.4471  0.0033 -0.1921 -0.0425 -0.1319
                                        0.0242 -0.0742 -0.0770 -0.0127
775. (0.00015) RY*( 4) C  40          s(  9.06%)p 6.78( 61.40%)d 3.26( 29.54%)
                                        0.0000  0.0023  0.2555 -0.1586 -0.0125
                                        0.0037 -0.1546 -0.3276  0.0024  0.0635
                                        0.1366  0.0092 -0.3435 -0.5848  0.1676
                                        0.0460  0.4984 -0.1295 -0.0031
776. (0.00010) RY*( 5) C  40          s( 14.09%)p 5.49( 77.32%)d 0.61(  8.59%)
777. (0.00007) RY*( 6) C  40          s( 47.62%)p 0.71( 33.79%)d 0.39( 18.59%)
778. (0.00002) RY*( 7) C  40          s( 69.33%)p 0.33( 22.96%)d 0.11(  7.71%)
779. (0.00002) RY*( 8) C  40          s(  0.62%)p86.32( 53.59%)d73.77( 45.79%)
780. (0.00003) RY*( 9) C  40          s(  5.65%)p 8.33( 47.09%)d 8.36( 47.26%)
781. (0.00001) RY*(10) C  40          s( 13.98%)p 3.66( 51.12%)d 2.50( 34.90%)
782. (0.00001) RY*(11) C  40          s(  4.66%)p 1.37(  6.41%)d19.08( 88.93%)
783. (0.00000) RY*(12) C  40          s( 99.25%)p 0.01(  0.69%)d 0.00(  0.07%)
784. (0.00000) RY*(13) C  40          s(  3.98%)p 2.83( 11.27%)d21.31( 84.75%)
785. (0.00000) RY*(14) C  40          s(  4.56%)p 1.36(  6.21%)d19.55( 89.22%)
786. (0.00651) RY*( 1) C  41          s(  5.88%)p14.80( 87.00%)d 1.21(  7.12%)
                                        0.0000  0.0079  0.2353  0.0582  0.0016
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                                     0.0079  0.4223 -0.0312 -0.0168 -0.7828
                                     0.0399 -0.0049 -0.2749  0.0211 -0.0686
                                    -0.1235  0.0703 -0.1473 -0.1567
787. (0.00320) RY*( 2) C  41        s(  0.33%)p99.99( 95.23%)d13.50(  4.44%)
                                     0.0000 -0.0021  0.0550 -0.0152 -0.0045
                                     0.0004 -0.7924 -0.0295  0.0009 -0.4939
                                    -0.0823 -0.0024  0.2675 -0.0356 -0.1747
                                    -0.0789  0.0252  0.0832 -0.0090
788. (0.00141) RY*( 3) C  41        s(  8.69%)p 8.73( 75.84%)d 1.78( 15.47%)
                                     0.0000 -0.0036  0.2789  0.0953  0.0004
                                     0.0021 -0.3207 -0.2796 -0.0066  0.1316
                                     0.3541  0.0046 -0.6283 -0.1996  0.1993
                                     0.0544  0.3066  0.1278  0.0411
789. (0.00100) RY*( 4) C  41        s( 33.88%)p 1.43( 48.39%)d 0.52( 17.73%)
                                     0.0000 -0.0043  0.5820  0.0091 -0.0019
                                     0.0052  0.0328 -0.0775 -0.0017  0.0753
                                     0.5524 -0.0086  0.3022  0.2730 -0.1055
                                     0.0259 -0.3840 -0.0274  0.1317
790. (0.00082) RY*( 5) C  41        s( 48.71%)p 0.17(  8.48%)d 0.88( 42.81%)
                                     0.0000  0.0014 -0.4201  0.5574 -0.0014
                                     0.0065 -0.0294 -0.1637 -0.0032 -0.0499
                                     0.2282 -0.0001 -0.0475  0.0148 -0.0604
                                    -0.3797 -0.1420 -0.2663  0.4349
791. (0.00072) RY*( 6) C  41        s( 32.40%)p 0.61( 19.73%)d 1.48( 47.87%)
                                     0.0000  0.0000 -0.2628  0.5049  0.0009
                                    -0.0053 -0.0079  0.1322 -0.0067 -0.0683
                                     0.3275 -0.0020  0.1318  0.2244  0.1003
                                     0.3272  0.1008  0.2609 -0.5323
792. (0.00041) RY*( 7) C  41        s( 47.56%)p 0.84( 40.04%)d 0.26( 12.40%)
                                     0.0000  0.0016  0.4279  0.5408  0.0054
                                     0.0044 -0.0448  0.2935  0.0013  0.0879
                                    -0.3456 -0.0037  0.0516 -0.4270  0.2186
                                     0.0134 -0.2205 -0.1453 -0.0795
793. (0.00039) RY*( 8) C  41        s( 16.45%)p 3.57( 58.67%)d 1.51( 24.89%)
                                     0.0000  0.0034  0.2473  0.3214 -0.0024
                                    -0.0088  0.0614 -0.3680 -0.0065  0.1544
                                    -0.4646  0.0025 -0.0462  0.4534 -0.2863
                                    -0.1751  0.1515  0.3366 -0.0033
794. (0.00033) RY*( 9) C  41        s(  1.10%)p70.47( 77.60%)d19.34( 21.30%)
                                     0.0000 -0.0017  0.1044 -0.0067  0.0080
                                     0.0081 -0.1697  0.6065  0.0010  0.0144
                                    -0.0395  0.0042 -0.1871  0.5853  0.2587
                                    -0.1290  0.2339 -0.2017  0.1844
795. (0.00014) RY*(10) C  41        s(  0.58%)p17.13(  9.85%)d99.99( 89.57%)
                                     0.0000 -0.0073  0.0725 -0.0149  0.0147
                                     0.0090 -0.0932 -0.0843 -0.0218  0.2630
                                     0.0833 -0.0051  0.0764 -0.0126 -0.3249
                                    -0.2432  0.2869 -0.6291 -0.5029
796. (0.00010) RY*(11) C  41        s(  0.28%)p99.99( 40.29%)d99.99( 59.43%)
797. (0.00005) RY*(12) C  41        s(  2.60%)p 0.32(  0.83%)d37.17( 96.57%)
798. (0.00000) RY*(13) C  41        s( 99.72%)p 0.00(  0.04%)d 0.00(  0.24%)
799. (0.00502) RY*( 1) C  42        s(  0.67%)p99.99( 92.55%)d10.07(  6.78%)
                                     0.0000  0.0021  0.0561  0.0597 -0.0033
                                     0.0129 -0.5020  0.0126 -0.0091  0.3133
                                    -0.0229  0.0198 -0.7576 -0.0056 -0.1290
                                     0.0543 -0.1935  0.0543 -0.0881
800. (0.00306) RY*( 2) C  42        s(  2.84%)p30.97( 87.97%)d 3.23(  9.19%)
                                     0.0000 -0.0019  0.1603 -0.0520  0.0017
                                     0.0023  0.0749 -0.0068  0.0002  0.8812
                                     0.0619  0.0026  0.3040 -0.0356  0.1123
                                     0.1884  0.0329  0.1635  0.1262
801. (0.00236) RY*( 3) C  42        s(  6.70%)p12.43( 83.31%)d 1.49(  9.99%)
                                     0.0000  0.0021  0.2563  0.0359  0.0048
                                    -0.0004 -0.7481 -0.0434  0.0045 -0.1261
                                    -0.1379  0.0027  0.4795  0.0817  0.1016
                                     0.0095 -0.2127 -0.1722  0.1208
802. (0.00137) RY*( 4) C  42        s( 87.22%)p 0.13( 11.67%)d 0.01(  1.11%)
                                     0.0000 -0.0032  0.9289 -0.0962 -0.0051
                                    -0.0028  0.2128  0.0186  0.0072 -0.1317
                                     0.1194 -0.0087 -0.1510  0.1286  0.0046
                                     0.0154  0.0654 -0.0482 -0.0651
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803. (0.00065) RY*( 5) C  42          s(  4.31%)p 5.56( 23.98%)d16.62( 71.70%)
                                        0.0000 -0.0041  0.1415  0.1516  0.0106
                                       -0.0084  0.0197  0.2782  0.0054  0.0582
                                       -0.3177  0.0067  0.0721 -0.2290 -0.5432
                                       -0.5074  0.0415  0.2261  0.3342
804. (0.00050) RY*( 6) C  42          s( 16.49%)p 4.06( 66.92%)d 1.01( 16.59%)
                                        0.0000 -0.0013 -0.0023  0.4056  0.0205
                                       -0.0020  0.0870  0.3418 -0.0002  0.0381
                                       -0.5158  0.0067  0.0438  0.5247  0.0643
                                        0.1796  0.0515  0.1244 -0.3337
805. (0.00042) RY*( 7) C  42          s(  2.63%)p21.99( 57.85%)d15.02( 39.52%)
                                        0.0000  0.0067 -0.0855  0.1376 -0.0026
                                        0.0054 -0.0099  0.1673 -0.0161 -0.0804
                                        0.4644 -0.0073 -0.0647  0.5691  0.0566
                                       -0.0492 -0.1263  0.2550  0.5555
806. (0.00033) RY*( 8) C  42          s( 68.01%)p 0.35( 23.55%)d 0.12(  8.45%)
                                        0.0000  0.0015  0.1024  0.8179 -0.0250
                                       -0.0007  0.1323 -0.3613  0.0062 -0.0210
                                        0.0442 -0.0072 -0.0437 -0.2881  0.2032
                                        0.0180 -0.1494 -0.0373  0.1384
807. (0.00024) RY*( 9) C  42          s(  1.29%)p15.64( 20.23%)d60.67( 78.47%)
                                        0.0000  0.0028  0.0403  0.1063 -0.0035
                                       -0.0170 -0.2698 -0.1523 -0.0073 -0.1701
                                        0.2270  0.0023  0.1094 -0.1164 -0.1482
                                        0.1982  0.4584  0.6768 -0.2353
808. (0.00013) RY*(10) C  42          s(  2.19%)p 4.03(  8.83%)d40.58( 88.97%)
                                        0.0000 -0.0004 -0.0293  0.1447 -0.0109
                                       -0.0070 -0.1844  0.0095  0.0049  0.1477
                                        0.0706 -0.0079 -0.0993  0.1322  0.2081
                                       -0.3574  0.7553 -0.3800  0.0622
809. (0.00012) RY*(11) C  42          s(  3.52%)p 9.29( 32.70%)d18.12( 63.78%)
                                        0.0000  0.0055 -0.0357  0.1837 -0.0114
                                       -0.0009  0.0072 -0.1017  0.0141  0.1637
                                        0.4419  0.0107  0.2076  0.2262 -0.4255
                                       -0.3283 -0.2080 -0.1857 -0.5208
810. (0.00007) RY*(12) C  42          s(  3.33%)p26.31( 87.69%)d 2.69(  8.98%)
811. (0.00004) RY*(13) C  42          s(  1.23%)p 2.24(  2.76%)d78.12( 96.02%)
812. (0.00000) RY*(14) C  42          s( 99.59%)p 0.00(  0.12%)d 0.00(  0.29%)
813. (0.00409) RY*( 1) C  43          s(  1.68%)p53.23( 89.18%)d 5.46(  9.15%)
                                        0.0000  0.0056  0.1292 -0.0045  0.0028
                                        0.0065  0.1931 -0.0591  0.0072  0.3803
                                        0.1272  0.0229  0.8304 -0.0052  0.1720
                                        0.0065  0.1764  0.0224  0.1738
814. (0.00153) RY*( 2) C  43          s(  0.24%)p99.99( 96.65%)d13.20(  3.12%)
                                        0.0000  0.0047  0.0469 -0.0101  0.0064
                                        0.0154  0.2250 -0.1894 -0.0121  0.8200
                                       -0.0722  0.0005 -0.4324  0.1231  0.0904
                                        0.1224 -0.0591 -0.0450 -0.0498
815. (0.00136) RY*( 3) C  43          s(  0.02%)p99.99( 96.34%)d99.99(  3.64%)
                                        0.0000  0.0039  0.0062  0.0091  0.0055
                                        0.0106 -0.8822  0.1356 -0.0209  0.3501
                                        0.1957  0.0068  0.0437 -0.0580 -0.1497
                                       -0.0314 -0.0198  0.0962  0.0584
816. (0.00060) RY*( 4) C  43          s( 92.59%)p 0.05(  4.74%)d 0.03(  2.67%)
                                        0.0000 -0.0002  0.9520 -0.1396 -0.0064
                                       -0.0123 -0.0228 -0.1041  0.0041 -0.1127
                                        0.0964 -0.0182 -0.0990 -0.0611  0.0107
                                        0.0272 -0.0782  0.1389 -0.0219
817. (0.00047) RY*( 5) C  43          s(  0.28%)p22.99(  6.33%)d99.99( 93.40%)
                                        0.0000  0.0008  0.0480 -0.0194 -0.0085
                                       -0.0061 -0.1761 -0.1493 -0.0049 -0.0727
                                        0.0081  0.0030  0.0566  0.0367  0.3784
                                        0.0244 -0.4414 -0.7543  0.1624
818. (0.00015) RY*( 6) C  43          s(  7.91%)p 5.73( 45.33%)d 5.91( 46.76%)
                                        0.0000 -0.0072  0.2023  0.1933 -0.0277
                                        0.0081 -0.0585  0.2357 -0.0163  0.1095
                                       -0.5708 -0.0056 -0.0175 -0.2365 -0.0441
                                       -0.4044  0.4195 -0.3490 -0.0655
819. (0.00012) RY*( 7) C  43          s(  2.81%)p15.50( 43.49%)d19.14( 53.71%)
                                        0.0000 -0.0090  0.0733  0.1490  0.0201
                                       -0.0103  0.1013  0.4708  0.0101  0.0859
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                                      -0.4214 -0.0093  0.1301 -0.0283 -0.2406
                                       0.2667 -0.5582  0.1523  0.2708
820. (0.00007) RY*( 8) C  43          s(  8.40%)p 6.96( 58.46%)d 3.95( 33.15%)
821. (0.00006) RY*( 9) C  43          s(  6.28%)p13.93( 87.46%)d 1.00(  6.27%)
822. (0.00005) RY*(10) C  43          s( 13.19%)p 1.19( 15.66%)d 5.40( 71.15%)
823. (0.00002) RY*(11) C  43          s( 66.65%)p 0.20( 13.54%)d 0.30( 19.81%)
824. (0.00002) RY*(12) C  43          s(  1.33%)p23.71( 31.42%)d50.75( 67.25%)
825. (0.00002) RY*(13) C  43          s(  2.08%)p 5.38( 11.18%)d41.77( 86.75%)
826. (0.00000) RY*(14) C  43          s( 96.61%)p 0.00(  0.39%)d 0.03(  3.00%)
827. (0.00417) RY*( 1) C  44          s(  0.90%)p99.99( 91.01%)d 9.00(  8.09%)
                                       0.0000  0.0007  0.0821  0.0471  0.0059
                                      -0.0114 -0.3280  0.0179  0.0292  0.8707
                                      -0.0564  0.0081  0.1994 -0.0092 -0.0770
                                      -0.1534  0.0616 -0.1314 -0.1743
828. (0.00187) RY*( 2) C  44          s(  0.05%)p99.99( 99.95%)d 0.09(  0.00%)
                                       0.0000 -0.0002  0.0193  0.0090  0.0007
                                      -0.0196  0.4821  0.1537  0.0008 -0.0088
                                      -0.0115 -0.0344  0.8157  0.2762  0.0017
                                      -0.0018  0.0009 -0.0049  0.0033
829. (0.00089) RY*( 3) C  44          s(  0.25%)p99.99( 91.27%)d34.04(  8.49%)
                                       0.0000  0.0014  0.0361  0.0345 -0.0016
                                       0.0057  0.7342 -0.1664  0.0014  0.3734
                                      -0.0821 -0.0025 -0.4353  0.1011  0.1796
                                       0.1509 -0.0367 -0.1174 -0.1213
830. (0.00051) RY*( 4) C  44          s( 98.54%)p 0.01(  1.35%)d 0.00(  0.11%)
                                       0.0000 -0.0013  0.9833  0.1357  0.0058
                                       0.0057 -0.0107  0.0204 -0.0158 -0.0837
                                       0.0710 -0.0035 -0.0244  0.0065 -0.0012
                                       0.0143 -0.0011  0.0211  0.0215
831. (0.00051) RY*( 5) C  44          s(  0.12%)p11.67(  1.38%)d99.99( 98.50%)
                                       0.0000  0.0006 -0.0003  0.0341 -0.0041
                                       0.0076  0.0885 -0.0316  0.0043  0.0464
                                       0.0077 -0.0043 -0.0514 -0.0005 -0.1609
                                      -0.4425 -0.3922 -0.4267  0.6538
832. (0.00020) RY*( 6) C  44          s(  0.08%)p99.99( 33.81%)d99.99( 66.12%)
                                       0.0000  0.0017  0.0059  0.0266 -0.0040
                                      -0.0165  0.0893 -0.2932  0.0014  0.0055
                                       0.0599 -0.0285  0.1549 -0.4642  0.3904
                                      -0.1528  0.6276 -0.1044  0.2840
833. (0.00008) RY*( 7) C  44          s( 41.20%)p 1.33( 54.63%)d 0.10(  4.17%)
834. (0.00007) RY*( 8) C  44          s(  7.39%)p 8.92( 65.87%)d 3.62( 26.74%)
835. (0.00004) RY*( 9) C  44          s(  0.08%)p99.99( 63.70%)d99.99( 36.22%)
836. (0.00004) RY*(10) C  44          s(  1.29%)p19.75( 25.49%)d56.75( 73.22%)
837. (0.00001) RY*(11) C  44          s( 48.03%)p 0.84( 40.34%)d 0.24( 11.64%)
838. (0.00000) RY*(12) C  44          s( 98.37%)p 0.01(  0.61%)d 0.01(  1.02%)
839. (0.00000) RY*(13) C  44          s(  0.20%)p78.03( 15.42%)d99.99( 84.38%)
840. (0.00000) RY*(14) C  44          s(  3.58%)p 4.28( 15.32%)d22.68( 81.10%)
841. (0.00417) RY*( 1) C  45          s(  1.43%)p62.69( 89.66%)d 6.23(  8.91%)
                                       0.0000  0.0053  0.1182 -0.0167  0.0039
                                      -0.0151 -0.5625 -0.0287  0.0101  0.4208
                                       0.1189 -0.0174 -0.6196  0.0598 -0.0762
                                       0.1114 -0.2438  0.1055 -0.0182
842. (0.00144) RY*( 2) C  45          s(  0.30%)p99.99( 98.57%)d 3.75(  1.13%)
                                       0.0000  0.0074  0.0535  0.0030  0.0083
                                       0.0043  0.0071 -0.0731 -0.0226  0.8154
                                       0.0686 -0.0182  0.5562  0.0237  0.0441
                                       0.0359  0.0447 -0.0089  0.0772
843. (0.00134) RY*( 3) C  45          s(  0.05%)p99.99( 92.47%)d99.99(  7.48%)
                                       0.0000 -0.0001  0.0225  0.0013  0.0008
                                       0.0121  0.7149 -0.2526  0.0088  0.2859
                                      -0.1745 -0.0031 -0.4569  0.1693  0.1251
                                       0.0276 -0.1167 -0.2111  0.0143
844. (0.00061) RY*( 4) C  45          s( 93.70%)p 0.04(  3.85%)d 0.03(  2.45%)
                                       0.0000 -0.0008  0.9598 -0.1251 -0.0048
                                       0.0088  0.0674  0.0830  0.0031 -0.1055
                                       0.0454  0.0222  0.0458  0.1061  0.0879
                                      -0.0481  0.0310  0.0714  0.0916
845. (0.00049) RY*( 5) C  45          s(  0.19%)p33.10(  6.26%)d99.99( 93.55%)
                                       0.0000  0.0005  0.0416 -0.0101 -0.0079
                                       0.0071 -0.1613 -0.0866  0.0030 -0.0858
                                      -0.0372 -0.0033  0.1063  0.0947  0.5591
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                                      0.5137 -0.0378 -0.2930 -0.5213
846. (0.00015) RY*( 6) C  45          s(  2.43%)p11.78( 28.60%)d28.41( 68.97%)
                                      0.0000 -0.0059  0.1359  0.0750 -0.0125
                                      0.0066 -0.0344  0.1662 -0.0190  0.0741
                                     -0.4907 -0.0093  0.1015  0.0138 -0.5021
                                     -0.1905 -0.2364 -0.2321 -0.5399
847. (0.00010) RY*( 7) C  45          s(  8.48%)p 8.40( 71.20%)d 2.40( 20.32%)
848. (0.00008) RY*( 8) C  45          s(  3.67%)p20.43( 74.95%)d 5.83( 21.38%)
849. (0.00005) RY*( 9) C  45          s(  1.91%)p18.19( 34.70%)d33.24( 63.40%)
850. (0.00006) RY*(10) C  45          s( 46.36%)p 0.59( 27.24%)d 0.57( 26.40%)
851. (0.00002) RY*(11) C  45          s(  1.11%)p24.38( 27.07%)d64.69( 71.82%)
852. (0.00002) RY*(12) C  45          s( 36.32%)p 0.81( 29.32%)d 0.95( 34.36%)
853. (0.00001) RY*(13) C  45          s(  6.71%)p 2.40( 16.12%)d11.49( 77.17%)
854. (0.00000) RY*(14) C  45          s( 97.38%)p 0.00(  0.13%)d 0.03(  2.49%)
855. (0.00513) RY*( 1) C  46          s(  0.59%)p99.99( 92.46%)d11.68(  6.95%)
                                      0.0000  0.0008  0.0028  0.0770 -0.0034
                                     -0.0103  0.3985 -0.0093 -0.0068  0.1200
                                     -0.0139 -0.0216  0.8660 -0.0214  0.1092
                                     -0.0499  0.2142 -0.0538  0.0792
856. (0.00295) RY*( 2) C  46          s(  4.53%)p19.27( 87.27%)d 1.81(  8.20%)
                                      0.0000 -0.0005  0.2128 -0.0002  0.0056
                                     -0.0047 -0.2665  0.0292  0.0020  0.8947
                                      0.0191 -0.0039  0.0009  0.0057  0.0894
                                      0.1064 -0.0803  0.1085  0.2108
857. (0.00289) RY*( 3) C  46          s(  0.12%)p99.99( 91.04%)d74.00(  8.84%)
                                      0.0000  0.0024  0.0344 -0.0027  0.0010
                                     -0.0037 -0.8188 -0.0944  0.0008 -0.2471
                                     -0.0422  0.0007  0.4090  0.0308  0.1293
                                      0.1789  0.0639  0.0819 -0.1698
858. (0.00146) RY*( 4) C  46          s( 93.19%)p 0.05(  4.68%)d 0.02(  2.13%)
                                      0.0000 -0.0036  0.9636 -0.0578 -0.0046
                                      0.0036  0.0905 -0.0185  0.0102 -0.1757
                                      0.0811  0.0076 -0.0043  0.0248 -0.0007
                                      0.0028 -0.0390 -0.1214 -0.0712
859. (0.00067) RY*( 5) C  46          s(  1.21%)p10.85( 13.12%)d70.87( 85.67%)
                                      0.0000 -0.0030  0.1044  0.0342  0.0030
                                      0.0113  0.0737  0.2571  0.0129  0.0698
                                     -0.2283 -0.0062 -0.0483  0.0011 -0.3126
                                      0.0305  0.4635  0.6428 -0.3606
860. (0.00052) RY*( 6) C  46          s( 49.12%)p 0.86( 42.45%)d 0.17(  8.44%)
                                      0.0000  0.0008  0.0916  0.6948  0.0100
                                     -0.0090 -0.0915 -0.1803  0.0038 -0.0131
                                     -0.4390  0.0039 -0.0623 -0.4321 -0.0459
                                     -0.2524  0.0031 -0.0772  0.1121
861. (0.00049) RY*( 7) C  46          s(  6.60%)p 9.94( 65.62%)d 4.21( 27.78%)
                                      0.0000  0.0060  0.0037  0.2568 -0.0033
                                      0.0097  0.0855 -0.3849 -0.0130 -0.0909
                                      0.6503 -0.0023 -0.0326 -0.2613  0.0902
                                      0.1734 -0.0013  0.4740  0.1223
862. (0.00029) RY*( 8) C  46          s( 32.11%)p 1.81( 58.18%)d 0.30(  9.70%)
                                      0.0000 -0.0012  0.0186  0.5660 -0.0197
                                      0.0034  0.0367  0.2350 -0.0012 -0.1022
                                      0.0127  0.0061 -0.0185  0.7171  0.0978
                                      0.1745 -0.1087  0.1036  0.1857
863. (0.00020) RY*( 9) C  46          s(  4.24%)p 1.86(  7.90%)d20.74( 87.87%)
                                      0.0000  0.0003 -0.0478  0.2002 -0.0024
                                      0.0090  0.1673  0.0075  0.0082  0.1456
                                     -0.0185 -0.0066 -0.1282 -0.1129  0.4961
                                      0.4185  0.0613 -0.2343 -0.6315
864. (0.00012) RY*(10) C  46          s(  7.89%)p 4.25( 33.53%)d 7.43( 58.58%)
                                      0.0000 -0.0016 -0.0503  0.2763 -0.0043
                                     -0.0049 -0.1381  0.1637  0.0120  0.1677
                                      0.5004  0.0082  0.0973  0.0346 -0.4943
                                     -0.2772 -0.0296 -0.3205 -0.4012
865. (0.00013) RY*(11) C  46          s(  0.06%)p99.99( 13.51%)d99.99( 86.42%)
                                      0.0000  0.0026  0.0156  0.0188  0.0056
                                     -0.0096 -0.1407  0.1286  0.0078 -0.0138
                                      0.2297 -0.0090 -0.2071  0.0521  0.3747
                                     -0.3299  0.7330 -0.1858  0.2077
866. (0.00009) RY*(12) C  46          s(  0.18%)p99.99( 88.64%)d62.84( 11.19%)
867. (0.00004) RY*(13) C  46          s(  0.88%)p 1.89(  1.66%)d99.99( 97.46%)
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868. (0.00000) RY*(14) C  46          s( 99.31%)p 0.00(  0.09%)d 0.01(  0.60%)
869. (0.00368) RY*( 1) C  47          s(  3.26%)p27.42( 89.38%)d 2.26(  7.36%)
                                        0.0000  0.0044  0.1686  0.0641  0.0056
                                        0.0114  0.3203 -0.0017 -0.0171 -0.7473
                                        0.0508 -0.0185 -0.4784 -0.0236 -0.1828
                                       -0.1742  0.0778 -0.0397 -0.0465
870. (0.00178) RY*( 2) C  47          s(  1.73%)p49.16( 84.84%)d 7.78( 13.43%)
                                        0.0000  0.0081  0.1088  0.0727 -0.0081
                                        0.0054  0.6638 -0.0790 -0.0017 -0.0729
                                       -0.0066  0.0023  0.6240  0.0822  0.1647
                                       -0.0809  0.2569  0.0463 -0.1804
871. (0.00140) RY*( 3) C  47          s(  5.62%)p14.14( 79.52%)d 2.64( 14.85%)
                                        0.0000  0.0005  0.2278  0.0658 -0.0021
                                        0.0013  0.4694 -0.0873 -0.0048  0.5747
                                       -0.0757 -0.0065 -0.4807 -0.0110 -0.1880
                                        0.2029  0.2353  0.0525  0.1179
872. (0.00067) RY*( 4) C  47          s( 29.33%)p 1.80( 52.91%)d 0.61( 17.76%)
                                        0.0000  0.0009  0.4852  0.2369 -0.0415
                                        0.0118 -0.2778  0.3842 -0.0069  0.0046
                                       -0.4480 -0.0086  0.0620  0.3154  0.0069
                                       -0.2593  0.2854  0.1097  0.1298
873. (0.00059) RY*( 5) C  47          s(  3.11%)p22.96( 71.45%)d 8.17( 25.44%)
                                        0.0000  0.0027  0.0968  0.1474 -0.0059
                                       -0.0045  0.1378  0.5300 -0.0085  0.1446
                                        0.6227  0.0040  0.0109  0.0754  0.0726
                                       -0.2095 -0.1463 -0.3513  0.2457
874. (0.00042) RY*( 6) C  47          s( 26.93%)p 1.57( 42.24%)d 1.14( 30.83%)
                                        0.0000 -0.0005  0.5139  0.0626  0.0364
                                        0.0038 -0.2329 -0.2202 -0.0016 -0.0344
                                        0.5520 -0.0077  0.0774 -0.0876 -0.0177
                                        0.1474  0.0589  0.5274 -0.0684
875. (0.00029) RY*( 7) C  47          s(  3.09%)p11.37( 35.19%)d19.95( 61.72%)
                                        0.0000  0.0028 -0.0533  0.1582  0.0553
                                       -0.0126  0.1074 -0.3229  0.0066 -0.1060
                                       -0.0307 -0.0061  0.1586  0.4456 -0.2475
                                        0.0667 -0.3392  0.1134  0.6508
876. (0.00030) RY*( 8) C  47          s( 25.69%)p 1.24( 31.98%)d 1.65( 42.32%)
                                        0.0000 -0.0006  0.4575 -0.2171 -0.0208
                                        0.0083 -0.1118 -0.4845 -0.0093  0.0600
                                       -0.0536 -0.0037  0.0843 -0.2427  0.0520
                                       -0.2848 -0.0125 -0.5592  0.1631
877. (0.00023) RY*( 9) C  47          s( 17.68%)p 2.40( 42.42%)d 2.26( 39.90%)
                                        0.0000  0.0019  0.0234  0.4195  0.0178
                                       -0.0056 -0.0581 -0.3108  0.0029  0.0940
                                        0.0701  0.0106 -0.2175  0.5128  0.3253
                                       -0.0422 -0.1937 -0.1950 -0.4646
878. (0.00013) RY*(10) C  47          s(  8.72%)p 0.99(  8.62%)d 9.47( 82.65%)
                                        0.0000 -0.0002  0.1247  0.2673  0.0162
                                        0.0061 -0.1260  0.0850  0.0171 -0.1580
                                        0.0012 -0.0138  0.1939 -0.0083 -0.3392
                                        0.6888  0.1554 -0.4504 -0.1007
879. (0.00011) RY*(11) C  47          s( 59.19%)p 0.59( 34.75%)d 0.10(  6.06%)
                                        0.0000 -0.0039 -0.1327  0.7578  0.0034
                                       -0.0024 -0.0094 -0.0949 -0.0006  0.0182
                                       -0.1016  0.0075  0.0254 -0.5719  0.0925
                                       -0.1432 -0.0478  0.0727  0.1549
880. (0.00011) RY*(12) C  47          s( 10.61%)p 1.52( 16.10%)d 6.91( 73.29%)
                                        0.0000  0.0005  0.3237 -0.0252  0.0264
                                       -0.0140  0.1704  0.2000 -0.0063  0.0851
                                       -0.2270 -0.0147  0.0961 -0.1532 -0.2866
                                       -0.0186 -0.7357  0.0843 -0.3195
881. (0.00003) RY*(13) C  47          s(  5.74%)p 1.84( 10.57%)d14.58( 83.69%)
882. (0.00000) RY*(14) C  47          s( 99.24%)p 0.00(  0.26%)d 0.01(  0.50%)
883. (0.00153) RY*( 1) C  48          s(  7.84%)p 9.32( 73.02%)d 2.44( 19.14%)
                                        0.0000  0.0016 -0.1826  0.2121 -0.0069
                                        0.0005 -0.3424 -0.1236 -0.0046 -0.5815
                                       -0.0798 -0.0146 -0.5026  0.0177  0.2701
                                        0.1443  0.0279 -0.0712 -0.3029
884. (0.00099) RY*( 2) C  48          s(  0.29%)p99.99( 72.12%)d95.79( 27.59%)
                                        0.0000  0.0009 -0.0356  0.0402 -0.0002
                                        0.0126  0.6201 -0.0647 -0.0076 -0.5275
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                                     0.0443  0.0048  0.2225  0.0505 -0.0520
                                     0.2409 -0.3050 -0.3257  0.1267
885. (0.00029) RY*( 3) C  48       s( 16.79%)p 4.86( 81.62%)d 0.09(  1.59%)
                                     0.0000  0.0040 -0.2142  0.3492 -0.0039
                                     0.0089 -0.4128 -0.3349  0.0047 -0.1124
                                    -0.1753 -0.0043  0.6554  0.2463 -0.0529
                                    -0.0391 -0.0461  0.0472  0.0847
886. (0.00011) RY*( 4) C  48       s( 31.01%)p 1.61( 49.82%)d 0.62( 19.18%)
                                     0.0000  0.0034 -0.2577  0.4936 -0.0014
                                    -0.0077  0.4014  0.4346  0.0023  0.0889
                                    -0.3316 -0.0026  0.0270  0.1717  0.1861
                                    -0.1675  0.2892  0.1331 -0.1665
887. (0.00012) RY*( 5) C  48       s( 11.53%)p 7.21( 83.16%)d 0.46(  5.31%)
                                     0.0000 -0.0172  0.0485  0.3241  0.0876
                                     0.0002 -0.1399  0.2772 -0.0020 -0.1596
                                     0.0999  0.0015  0.1885 -0.8150 -0.1282
                                     0.1269  0.0818  0.0639  0.0989
888. (0.00007) RY*( 6) C  48       s( 25.60%)p 1.87( 47.80%)d 1.04( 26.60%)
889. (0.00004) RY*( 7) C  48       s( 16.12%)p 2.55( 41.05%)d 2.66( 42.83%)
890. (0.00003) RY*( 8) C  48       s( 71.48%)p 0.30( 21.49%)d 0.10(  7.03%)
891. (0.00002) RY*( 9) C  48       s(  7.05%)p 8.15( 57.43%)d 5.04( 35.52%)
892. (0.00000) RY*(10) C  48       s( 99.18%)p 0.01(  0.80%)d 0.00(  0.02%)
893. (0.00001) RY*(11) C  48       s(  4.86%)p 8.20( 39.82%)d11.39( 55.33%)
894. (0.00001) RY*(12) C  48       s(  6.40%)p 1.68( 10.72%)d12.96( 82.88%)
895. (0.00001) RY*(13) C  48       s(  1.31%)p11.68( 15.27%)d63.83( 83.42%)
896. (0.00000) RY*(14) C  48       s(  0.56%)p10.79(  6.06%)d99.99( 93.38%)
897. (0.00367) RY*( 1) C  49       s(  2.72%)p32.92( 89.61%)d 2.82(  7.66%)
                                     0.0000  0.0050  0.1621  0.0300  0.0044
                                     0.0161  0.4891 -0.0108 -0.0245 -0.8037
                                     0.0700  0.0052  0.0517  0.0484 -0.1794
                                    -0.0140  0.0864 -0.1576 -0.1093
898. (0.00133) RY*( 2) C  49       s(  0.46%)p99.99( 80.08%)d42.77( 19.46%)
                                     0.0000  0.0081  0.0026  0.0668  0.0035
                                     0.0019 -0.3569 -0.0730 -0.0069 -0.2436
                                    -0.0896 -0.0064 -0.7562 -0.1698 -0.0348
                                    -0.2950 -0.1552 -0.0040 -0.2868
899. (0.00128) RY*( 3) C  49       s(  0.19%)p99.99( 84.81%)d78.93( 15.00%)
                                     0.0000  0.0013  0.0407  0.0154  0.0015
                                    -0.0013  0.6688 -0.1938 -0.0002  0.3913
                                    -0.1225 -0.0002 -0.4296  0.1031 -0.0821
                                    -0.1433 -0.1662 -0.1827  0.2484
900. (0.00068) RY*( 4) C  49       s(  0.47%)p99.99( 62.30%)d80.04( 37.23%)
                                     0.0000 -0.0011  0.0665 -0.0153  0.0005
                                     0.0123 -0.3187 -0.4962  0.0061 -0.1652
                                    -0.2450 -0.0057  0.1812  0.3935 -0.2849
                                    -0.3090 -0.0973  0.0242  0.4308
901. (0.00050) RY*( 5) C  49       s( 54.24%)p 0.30( 16.24%)d 0.54( 29.52%)
                                     0.0000  0.0041  0.7303  0.0947 -0.0064
                                     0.0112 -0.0875 -0.1680 -0.0161  0.1511
                                    -0.0086  0.0019  0.0788 -0.3116 -0.3416
                                     0.3174 -0.2518 -0.0279 -0.1166
902. (0.00034) RY*( 6) C  49       s( 10.53%)p 7.64( 80.42%)d 0.86(  9.04%)
                                     0.0000 -0.0033  0.3045 -0.1096  0.0244
                                     0.0071 -0.1518  0.1038 -0.0020  0.0130
                                     0.5798  0.0085 -0.3166  0.5777  0.0693
                                     0.2228  0.1288 -0.0397  0.1335
903. (0.00026) RY*( 7) C  49       s( 15.97%)p 1.25( 19.98%)d 4.01( 64.05%)
                                     0.0000 -0.0018  0.3989 -0.0145 -0.0179
                                     0.0015  0.0473  0.3017 -0.0070  0.1185
                                     0.1980 -0.0081  0.2302 -0.0139  0.1515
                                    -0.7793 -0.0635  0.0058 -0.0792
904. (0.00027) RY*( 8) C  49       s(  1.72%)p21.54( 37.06%)d35.58( 61.22%)
                                     0.0000 -0.0017  0.1310  0.0072 -0.0004
                                    -0.0016  0.0365 -0.3534 -0.0039  0.0692
                                    -0.2639 -0.0062  0.1275  0.3920  0.4730
                                     0.0610 -0.0615 -0.2092 -0.5807
905. (0.00018) RY*( 9) C  49       s(  0.49%)p42.07( 20.47%)d99.99( 79.04%)
                                     0.0000  0.0027  0.0632  0.0292  0.0018
                                    -0.0165  0.1764 -0.3781 -0.0056  0.0986
                                     0.1266  0.0098 -0.0588 -0.0326 -0.0954
                                    -0.1042  0.4825  0.7004 -0.2170
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906. (0.00015) RY*(10) C  49          s(  1.20%)p39.39( 47.37%)d42.76( 51.43%)
                                        0.0000  0.0070  0.1075 -0.0195 -0.0059
                                        0.0043 -0.0415 -0.4382  0.0141 -0.1277
                                        0.2521  0.0078 -0.0180 -0.4467  0.5665
                                       -0.0099  0.1430 -0.1938  0.3677
907. (0.00009) RY*(11) C  49          s( 14.52%)p 3.36( 48.81%)d 2.52( 36.66%)
908. (0.00002) RY*(12) C  49          s(  1.63%)p 6.92( 11.25%)d53.56( 87.12%)
909. (0.00003) RY*(13) C  49          s( 96.02%)p 0.02(  1.67%)d 0.02(  2.31%)
910. (0.00000) RY*(14) C  49          s( 99.80%)p 0.00(  0.13%)d 0.00(  0.06%)
911. (0.00165) RY*( 1) C  50          s(  3.37%)p23.66( 79.69%)d 5.03( 16.95%)
                                        0.0000  0.0010 -0.1183  0.1402 -0.0053
                                        0.0060 -0.1020 -0.0779 -0.0074 -0.4681
                                        0.0122  0.0117  0.7483  0.0308  0.2271
                                       -0.3190 -0.1150 -0.0508  0.0184
912. (0.00104) RY*( 2) C  50          s(  2.20%)p34.75( 76.48%)d 9.69( 21.32%)
                                        0.0000 -0.0010  0.1055 -0.1042  0.0025
                                       -0.0030  0.0555  0.0875  0.0111  0.7034
                                       -0.0670  0.0079  0.5035 -0.0330 -0.3758
                                       -0.2404 -0.0630  0.0624 -0.0793
913. (0.00038) RY*( 3) C  50          s( 28.68%)p 2.48( 71.03%)d 0.01(  0.28%)
                                        0.0000 -0.0040  0.4061 -0.3489  0.0127
                                       -0.0151  0.7199  0.3426 -0.0010 -0.2591
                                        0.0237  0.0014  0.0795 -0.0204  0.0297
                                       -0.0258 -0.0023 -0.0341 -0.0112
914. (0.00016) RY*( 4) C  50          s( 10.21%)p 5.43( 55.42%)d 3.36( 34.36%)
                                        0.0000  0.0015  0.2870 -0.1396 -0.0170
                                       -0.0007 -0.0710 -0.2184 -0.0086  0.2536
                                        0.5343 -0.0071  0.2205  0.3209  0.4122
                                        0.3560  0.1619 -0.0515  0.1348
915. (0.00011) RY*( 5) C  50          s( 22.60%)p 2.81( 63.42%)d 0.62( 13.98%)
                                        0.0000  0.0168  0.3334 -0.3313 -0.0695
                                       -0.0023 -0.0478 -0.7229  0.0057 -0.1484
                                       -0.1724  0.0004  0.0015 -0.2398 -0.1085
                                       -0.0196  0.0160  0.2261 -0.2761
916. (0.00008) RY*( 6) C  50          s( 33.44%)p 1.63( 54.41%)d 0.36( 12.15%)
917. (0.00002) RY*( 7) C  50          s( 73.30%)p 0.26( 18.92%)d 0.11(  7.78%)
918. (0.00003) RY*( 8) C  50          s(  9.89%)p 3.21( 31.74%)d 5.90( 58.37%)
919. (0.00002) RY*( 9) C  50          s(  0.70%)p61.03( 42.96%)d80.02( 56.33%)
920. (0.00001) RY*(10) C  50          s(  0.52%)p99.99( 85.09%)d27.92( 14.39%)
921. (0.00000) RY*(11) C  50          s( 99.21%)p 0.01(  0.57%)d 0.00(  0.21%)
922. (0.00000) RY*(12) C  50          s(  0.22%)p37.56(  8.37%)d99.99( 91.41%)
923. (0.00001) RY*(13) C  50          s(  6.05%)p 1.29(  7.78%)d14.25( 86.17%)
924. (0.00001) RY*(14) C  50          s(  9.60%)p 0.45(  4.29%)d 8.97( 86.11%)
925. (0.00364) RY*( 1) C  51          s(  2.61%)p34.38( 89.60%)d 2.99(  7.79%)
                                        0.0000  0.0044  0.1586  0.0296  0.0029
                                       -0.0082 -0.3436  0.0799  0.0134  0.4970
                                       -0.0540  0.0248  0.7215 -0.0103 -0.1749
                                       -0.1447  0.1603  0.0110  0.0241
926. (0.00135) RY*( 2) C  51          s(  0.83%)p95.86( 79.35%)d23.95( 19.82%)
                                        0.0000  0.0083 -0.0022  0.0903  0.0067
                                       -0.0077 -0.6082 -0.1999  0.0059  0.3194
                                        0.0172 -0.0003 -0.5245 -0.0787  0.1819
                                       -0.3428  0.0605 -0.2055 -0.0415
927. (0.00123) RY*( 3) C  51          s(  0.08%)p99.99( 88.14%)d99.99( 11.78%)
                                        0.0000 -0.0004  0.0285  0.0053 -0.0002
                                        0.0010 -0.5475  0.0826  0.0042 -0.7070
                                        0.1569  0.0023  0.2128 -0.0711  0.1505
                                        0.0520  0.2620  0.0894 -0.1258
928. (0.00063) RY*( 4) C  51          s(  0.18%)p99.99( 47.05%)d99.99( 52.76%)
                                        0.0000  0.0016  0.0429 -0.0001  0.0005
                                       -0.0084  0.1741  0.1870 -0.0100  0.2628
                                        0.5398  0.0060 -0.1000 -0.1861  0.3154
                                       -0.0569  0.3098  0.5661 -0.0919
929. (0.00048) RY*( 5) C  51          s( 57.09%)p 0.20( 11.55%)d 0.55( 31.36%)
                                        0.0000  0.0037  0.7488  0.1007 -0.0066
                                       -0.0049  0.1002 -0.1540  0.0112 -0.1117
                                       -0.0041  0.0164 -0.1081 -0.2391 -0.0779
                                        0.0206  0.2053 -0.0626  0.5109
930. (0.00035) RY*( 6) C  51          s(  5.66%)p14.47( 81.94%)d 2.19( 12.40%)
                                        0.0000 -0.0031  0.2090 -0.1103  0.0275
                                        0.0065 -0.2133  0.7207 -0.0028  0.0952
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                                      -0.4058  0.0074 -0.2822 -0.0313 -0.1068
                                       0.2542 -0.0595  0.2021 -0.0598
931. (0.00026) RY*( 7) C  51        s( 17.83%)p 0.78( 13.97%)d 3.83( 68.21%)
                                       0.0000 -0.0019  0.4220 -0.0085 -0.0084
                                      -0.0094  0.2408  0.2330  0.0067 -0.1216
                                      -0.0272 -0.0007  0.1038  0.0305  0.2791
                                      -0.5302 -0.2004 -0.2478 -0.4706
932. (0.00025) RY*( 8) C  51        s(  0.20%)p99.99( 60.23%)d99.99( 39.57%)
                                       0.0000 -0.0013  0.0422 -0.0161 -0.0003
                                      -0.0058  0.0773 -0.3247 -0.0011 -0.0244
                                      -0.6194  0.0003  0.0119  0.3263  0.3069
                                      -0.1261  0.3230  0.4224 -0.0530
933. (0.00018) RY*( 9) C  51        s(  0.22%)p42.96(  9.38%)d99.99( 90.40%)
                                       0.0000  0.0021  0.0460  0.0067 -0.0041
                                      -0.0099  0.1420 -0.0835 -0.0171  0.1467
                                      -0.0834  0.0044 -0.0296 -0.1921  0.0679
                                       0.4654  0.5310 -0.4335 -0.4615
934. (0.00013) RY*(10) C  51        s(  0.60%)p99.99( 61.14%)d64.19( 38.26%)
                                       0.0000  0.0073  0.0765 -0.0060 -0.0044
                                       0.0134 -0.0777 -0.3421 -0.0065  0.0151
                                      -0.1924 -0.0027  0.0884 -0.6656  0.0261
                                       0.1471 -0.4392  0.2999 -0.2783
935. (0.00010) RY*(11) C  51        s( 19.41%)p 2.20( 42.68%)d 1.95( 37.92%)
                                       0.0000 -0.0013  0.3936 -0.1954 -0.0304
                                       0.0095 -0.1402 -0.2851  0.0000  0.0426
                                       0.2808  0.0182 -0.1262  0.4784 -0.3744
                                       0.2019 -0.1355  0.1970 -0.3756
936. (0.00003) RY*(12) C  51        s( 93.08%)p 0.02(  2.07%)d 0.05(  4.85%)
937. (0.00002) RY*(13) C  51        s(  2.42%)p 5.36( 12.96%)d35.01( 84.63%)
938. (0.00000) RY*(14) C  51        s( 99.75%)p 0.00(  0.18%)d 0.00(  0.07%)
939. (0.00168) RY*( 1) C  52        s(  2.76%)p29.07( 80.38%)d 6.10( 16.86%)
                                       0.0000  0.0008 -0.0974  0.1347 -0.0050
                                       0.0022 -0.0697 -0.0099 -0.0019 -0.4739
                                      -0.0775  0.0148  0.7535 -0.0154  0.1404
                                      -0.2105 -0.2567 -0.1143 -0.1600
940. (0.00104) RY*( 2) C  52        s(  2.02%)p38.21( 77.10%)d10.35( 20.88%)
                                       0.0000 -0.0010  0.1021 -0.0987  0.0029
                                       0.0102  0.7770 -0.0218 -0.0084 -0.3778
                                       0.0889 -0.0037 -0.1088  0.0638 -0.1083
                                      -0.1219  0.2005 -0.3680  0.0812
941. (0.00037) RY*( 3) C  52        s( 26.52%)p 2.76( 73.13%)d 0.01(  0.35%)
                                       0.0000 -0.0043  0.3776 -0.3499  0.0124
                                      -0.0078  0.2215  0.1974 -0.0127  0.5600
                                       0.2732 -0.0044  0.4952  0.0981 -0.0138
                                      -0.0424 -0.0347  0.0131 -0.0118
942. (0.00017) RY*( 4) C  52        s( 11.77%)p 4.37( 51.46%)d 3.12( 36.77%)
                                       0.0000  0.0026  0.3227 -0.1149 -0.0188
                                      -0.0106  0.2501  0.3830  0.0048 -0.2271
                                      -0.4611  0.0000 -0.0448 -0.1976  0.0566
                                       0.2660 -0.1792  0.5029 -0.0935
943. (0.00011) RY*( 5) C  52        s( 21.30%)p 3.04( 64.75%)d 0.66( 13.96%)
                                       0.0000 -0.0167 -0.2438  0.3848  0.0717
                                      -0.0045  0.1044  0.5771  0.0031 -0.0434
                                       0.3809  0.0030 -0.0845  0.3865 -0.1825
                                       0.0166 -0.2818  0.1519  0.0591
944. (0.00008) RY*( 6) C  52        s( 38.07%)p 1.33( 50.63%)d 0.30( 11.30%)
945. (0.00002) RY*( 7) C  52        s( 78.24%)p 0.21( 16.46%)d 0.07(  5.30%)
946. (0.00001) RY*( 8) C  52        s(  1.19%)p81.77( 97.42%)d 1.16(  1.39%)
947. (0.00001) RY*( 9) C  52        s(  2.09%)p 4.11(  8.58%)d42.83( 89.33%)
948. (0.00001) RY*(10) C  52        s(  8.26%)p 1.12(  9.27%)d 9.99( 82.47%)
949. (0.00002) RY*(11) C  52        s(  3.33%)p14.52( 48.35%)d14.51( 48.32%)
950. (0.00002) RY*(12) C  52        s(  8.45%)p 2.22( 18.77%)d 8.61( 72.78%)
951. (0.00000) RY*(13) C  52        s( 95.86%)p 0.01(  0.64%)d 0.04(  3.50%)
952. (0.00001) RY*(14) C  52        s(  0.15%)p21.75(  3.25%)d99.99( 96.60%)
953. (0.00371) RY*( 1) C  53        s(  4.46%)p19.79( 88.30%)d 1.62(  7.24%)
                                       0.0000  0.0044  0.1987  0.0713  0.0061
                                      -0.0152 -0.5844  0.0110  0.0245  0.7011
                                      -0.0180  0.0016  0.2176 -0.0361 -0.1422
                                      -0.0978  0.1067 -0.1658 -0.0613
954. (0.00163) RY*( 2) C  53        s(  2.95%)p27.94( 82.54%)d 4.91( 14.51%)
                                       0.0000  0.0083  0.1627  0.0538 -0.0097
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                                      0.0016  0.6211 -0.0926  0.0056  0.2637
                                     -0.1273  0.0045  0.5843  0.0616 -0.0282
                                      0.0599  0.1413  0.1070 -0.3306
955. (0.00137) RY*( 3) C  53        s(  5.90%)p13.16( 77.64%)d 2.79( 16.46%)
                                      0.0000 -0.0013  0.2252  0.0902  0.0127
                                     -0.0038  0.3607 -0.0964  0.0024  0.4345
                                     -0.0827 -0.0026 -0.6599 -0.0761 -0.2242
                                      0.2835  0.0876  0.0536  0.1531
956. (0.00073) RY*( 4) C  53        s( 38.35%)p 1.20( 46.05%)d 0.41( 15.60%)
                                      0.0000  0.0019  0.5306  0.3175 -0.0345
                                     -0.0030 -0.0774  0.1056  0.0133 -0.2532
                                      0.1244  0.0036 -0.1050  0.5938 -0.1845
                                      0.0302 -0.1479 -0.1507 -0.2764
957. (0.00061) RY*( 5) C  53        s(  0.74%)p99.99( 74.46%)d33.51( 24.80%)
                                      0.0000 -0.0028  0.0769 -0.0364  0.0122
                                      0.0083 -0.2629 -0.7207  0.0061 -0.2003
                                     -0.3275 -0.0060 -0.0072  0.0919  0.1577
                                      0.3409  0.3097  0.0163 -0.1037
958. (0.00039) RY*( 6) C  53        s( 24.89%)p 1.92( 47.88%)d 1.09( 27.23%)
                                      0.0000 -0.0011  0.4825 -0.1258  0.0190
                                     -0.0048 -0.0593  0.4003  0.0098 -0.2085
                                     -0.0545 -0.0020  0.0671 -0.5137  0.2140
                                      0.3950  0.1474 -0.2058 -0.0797
959. (0.00032) RY*( 7) C  53        s(  9.32%)p 4.13( 38.45%)d 5.60( 52.23%)
                                      0.0000  0.0016  0.2980 -0.0615  0.0248
                                     -0.0051  0.0410 -0.1918  0.0016 -0.1203
                                     -0.5191 -0.0024  0.1362 -0.2085 -0.2935
                                     -0.2516 -0.5252 -0.1005  0.2948
960. (0.00029) RY*( 8) C  53        s( 13.15%)p 1.87( 24.65%)d 4.73( 62.20%)
                                      0.0000 -0.0028  0.3047 -0.1891 -0.0540
                                      0.0010 -0.0270 -0.2016  0.0107 -0.0883
                                      0.2059  0.0143 -0.2298 -0.3191 -0.0425
                                     -0.5567  0.1396  0.3450 -0.4144
961. (0.00021) RY*( 9) C  53        s( 12.18%)p 3.43( 41.78%)d 3.78( 46.04%)
                                      0.0000  0.0026  0.0298  0.3456  0.0378
                                      0.0001  0.0004  0.2557 -0.0147  0.0868
                                     -0.5485  0.0025 -0.1754  0.1141  0.5713
                                     -0.3170  0.1086  0.1457 -0.0220
962. (0.00013) RY*(10) C  53        s(  9.61%)p 1.11( 10.65%)d 8.30( 79.74%)
                                      0.0000  0.0002  0.1657  0.2602  0.0302
                                      0.0096 -0.1033  0.1323  0.0085 -0.1797
                                      0.0293 -0.0187  0.2113  0.0062 -0.3043
                                      0.0025  0.4134  0.5418  0.4902
963. (0.00010) RY*(11) C  53        s(  9.57%)p 2.96( 28.32%)d 6.49( 62.11%)
                                      0.0000 -0.0003  0.3086  0.0202  0.0057
                                     -0.0172  0.1901 -0.2816 -0.0004  0.0527
                                      0.3927 -0.0097  0.0817  0.0609  0.4177
                                     -0.2605  0.1231 -0.3427  0.4961
964. (0.00011) RY*(12) C  53        s( 63.64%)p 0.46( 29.07%)d 0.11(  7.29%)
                                      0.0000 -0.0038 -0.1321  0.7866  0.0120
                                      0.0053 -0.0164 -0.2188 -0.0069 -0.0499
                                      0.2111  0.0058  0.0413 -0.4401  0.0278
                                      0.0810 -0.2203 -0.0278 -0.1276
965. (0.00003) RY*(13) C  53        s(  5.90%)p 1.72( 10.15%)d14.22( 83.95%)
966. (0.00000) RY*(14) C  53        s( 99.28%)p 0.00(  0.32%)d 0.00(  0.41%)
967. (0.00150) RY*( 1) C  54        s(  6.65%)p11.17( 74.28%)d 2.87( 19.06%)
                                      0.0000  0.0015 -0.1563  0.2051 -0.0076
                                     -0.0090 -0.8186 -0.1223  0.0095  0.1317
                                     -0.0980 -0.0069 -0.1750 -0.0050  0.2065
                                     -0.0939  0.1127  0.3332 -0.1243
968. (0.00097) RY*( 2) C  54        s(  0.75%)p95.23( 71.17%)d37.58( 28.08%)
                                      0.0000  0.0010 -0.0525  0.0687 -0.0009
                                      0.0018 -0.0520  0.0149  0.0091  0.3931
                                     -0.1108  0.0131  0.7358 -0.0172 -0.0669
                                     -0.1448 -0.1436  0.2196  0.4319
969. (0.00026) RY*( 3) C  54        s( 16.75%)p 4.82( 80.81%)d 0.15(  2.45%)
                                      0.0000  0.0049 -0.2034  0.3551 -0.0042
                                      0.0067 -0.0462 -0.2533  0.0076 -0.6974
                                     -0.3655 -0.0027  0.3083  0.1633 -0.0257
                                      0.0563 -0.0427 -0.1364  0.0142
970. (0.00011) RY*( 4) C  54        s( 21.74%)p 3.37( 73.26%)d 0.23(  5.00%)
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                                      0.0000 -0.0157 -0.0446  0.4562  0.0841
                                     -0.0019 -0.0302 -0.0716 -0.0012 -0.1121
                                      0.7449  0.0003  0.1832 -0.3542 -0.0984
                                      0.1679  0.1003  0.0123 -0.0440
971. (0.00012) RY*( 5) C  54        s( 14.62%)p 4.19( 61.31%)d 1.65( 24.07%)
                                      0.0000  0.0075 -0.2044  0.3217 -0.0301
                                     -0.0032  0.2470  0.0470 -0.0046  0.3075
                                      0.1203 -0.0073  0.1257  0.6519  0.1268
                                     -0.0393  0.0858  0.0273 -0.4636
972. (0.00007) RY*( 6) C  54        s( 32.06%)p 1.38( 44.30%)d 0.74( 23.64%)
973. (0.00003) RY*( 7) C  54        s( 77.70%)p 0.14( 11.11%)d 0.14( 11.19%)
974. (0.00003) RY*( 8) C  54        s(  0.56%)p99.99( 91.54%)d14.10(  7.90%)
975. (0.00003) RY*( 9) C  54        s( 16.05%)p 1.40( 22.39%)d 3.83( 61.56%)
976. (0.00001) RY*(10) C  54        s(  1.39%)p 3.23(  4.48%)d67.94( 94.14%)
977. (0.00001) RY*(11) C  54        s(  1.94%)p 7.46( 14.50%)d42.96( 83.55%)
978. (0.00000) RY*(12) C  54        s(  6.36%)p 0.56(  3.57%)d14.17( 90.08%)
979. (0.00001) RY*(13) C  54        s(  4.29%)p10.88( 46.65%)d11.44( 49.07%)
980. (0.00000) RY*(14) C  54        s( 99.14%)p 0.01(  0.82%)d 0.00(  0.04%)
981. (0.00160) RY*( 1) C  55        s(  8.63%)p 8.47( 73.11%)d 2.12( 18.26%)
                                      0.0000 -0.0071  0.2627 -0.1314  0.0003
                                      0.0003  0.2914  0.1130 -0.0146 -0.0432
                                      0.1474 -0.0172 -0.7659 -0.1507 -0.1076
                                      0.1990  0.3499 -0.0473 -0.0821
982. (0.00113) RY*( 2) C  55        s(  2.58%)p30.66( 79.23%)d 7.04( 18.18%)
                                      0.0000 -0.0019  0.1290 -0.0958 -0.0033
                                     -0.0142 -0.6721  0.1256  0.0036  0.5352
                                      0.0342 -0.0027 -0.1924  0.0016  0.2924
                                      0.1034  0.0903  0.2779  0.0171
983. (0.00043) RY*( 3) C  55        s(  7.91%)p11.44( 90.47%)d 0.21(  1.63%)
                                      0.0000  0.0048 -0.0783  0.2701 -0.0012
                                      0.0064 -0.5202  0.0077  0.0102 -0.7159
                                     -0.2619 -0.0060 -0.2296  0.0022  0.0535
                                      0.0379  0.0995  0.0200 -0.0406
984. (0.00016) RY*( 4) C  55        s( 76.62%)p 0.25( 18.86%)d 0.06(  4.52%)
                                      0.0000  0.0064  0.6640 -0.5697 -0.0263
                                      0.0026 -0.1698 -0.0221  0.0004 -0.2481
                                     -0.0481 -0.0052  0.2820 -0.1259 -0.0267
                                      0.0098 -0.0713 -0.1722 -0.0980
985. (0.00015) RY*( 5) C  55        s(  0.32%)p99.99( 97.03%)d 8.21(  2.64%)
                                      0.0000 -0.0015  0.0554  0.0014  0.0121
                                     -0.0056  0.1541  0.9199  0.0008 -0.1021
                                     -0.0925 -0.0032  0.1091  0.2636  0.1298
                                      0.0215 -0.0437  0.0818  0.0233
986. (0.00009) RY*( 6) C  55        s(  3.69%)p23.98( 88.47%)d 2.12(  7.84%)
987. (0.00009) RY*( 7) C  55        s( 19.02%)p 1.02( 19.32%)d 3.24( 61.66%)
988. (0.00004) RY*( 8) C  55        s(  9.12%)p 8.09( 73.83%)d 1.87( 17.04%)
989. (0.00004) RY*( 9) C  55        s( 63.98%)p 0.23( 15.02%)d 0.33( 21.00%)
990. (0.00001) RY*(10) C  55        s(  1.35%)p 7.73( 10.41%)d65.53( 88.24%)
991. (0.00002) RY*(11) C  55        s(  0.71%)p28.29( 20.13%)d99.99( 79.16%)
992. (0.00000) RY*(12) C  55        s( 99.18%)p 0.01(  0.71%)d 0.00(  0.11%)
993. (0.00001) RY*(13) C  55        s(  4.27%)p 1.67(  7.13%)d20.73( 88.59%)
994. (0.00001) RY*(14) C  55        s(  2.62%)p 2.46(  6.44%)d34.76( 90.94%)
995. (0.00167) RY*( 1) C  56        s(  8.76%)p 8.44( 73.95%)d 1.97( 17.29%)
                                      0.0000 -0.0072  0.2790  0.0985 -0.0006
                                     -0.0120  0.0243  0.1433  0.0184  0.8349
                                      0.1281  0.0077 -0.0042 -0.0663 -0.3177
                                      0.0276  0.2293  0.1273  0.0496
996. (0.00111) RY*( 2) C  56        s(  2.23%)p36.36( 81.12%)d 7.46( 16.65%)
                                      0.0000 -0.0032  0.0974  0.1132 -0.0016
                                     -0.0093 -0.2570  0.0912 -0.0032 -0.0665
                                      0.0018 -0.0117 -0.8555  0.0154 -0.0071
                                      0.1594 -0.0387  0.2002 -0.3154
997. (0.00050) RY*( 3) C  56        s(  2.73%)p35.23( 96.09%)d 0.43(  1.18%)
                                      0.0000 -0.0060  0.0441  0.1590  0.0048
                                     -0.0109  0.9077  0.2141 -0.0045 -0.0771
                                      0.0334  0.0067 -0.2517 -0.1436  0.0465
                                      0.0094 -0.0418 -0.0752  0.0465
998. (0.00022) RY*( 4) C  56        s( 80.54%)p 0.21( 16.56%)d 0.04(  2.90%)
                                      0.0000  0.0076  0.6293  0.6394 -0.0242
                                     -0.0023 -0.0661 -0.2740  0.0024 -0.2625
                                      0.0420  0.0020  0.1240 -0.0079 -0.0348
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                                      -0.1246 -0.0151  0.0574  0.0935
 999. (0.00013) RY*( 5) C  56          s(  2.27%)p22.17( 50.43%)d20.79( 47.29%)
                                        0.0000  0.0000  0.0619  0.1361  0.0200
                                       -0.0095  0.0862  0.4238  0.0002 -0.0399
                                       -0.0955 -0.0107  0.3761  0.4062 -0.0091
                                        0.2037 -0.1882  0.3286 -0.5366
1000. (0.00010) RY*( 6) C  56          s(  9.31%)p 9.31( 86.70%)d 0.43(  3.99%)
                                        0.0000 -0.0127  0.2868 -0.0892  0.0526
                                       -0.0005 -0.2289  0.6088  0.0098 -0.1389
                                       -0.2782  0.0060  0.1013 -0.5805  0.0834
                                        0.0633  0.0028 -0.1518  0.0765
1001. (0.00004) RY*( 7) C  56          s(  5.89%)p15.45( 91.00%)d 0.53(  3.11%)
1002. (0.00005) RY*( 8) C  56          s( 11.22%)p 5.05( 56.71%)d 2.86( 32.07%)
1003. (0.00003) RY*( 9) C  56          s( 49.46%)p 0.50( 24.96%)d 0.52( 25.58%)
1004. (0.00001) RY*(10) C  56          s(  6.81%)p 1.33(  9.06%)d12.36( 84.14%)
1005. (0.00001) RY*(11) C  56          s(  0.25%)p 7.08(  1.79%)d99.99( 97.95%)
1006. (0.00001) RY*(12) C  56          s( 11.94%)p 0.42(  4.97%)d 6.96( 83.08%)
1007. (0.00001) RY*(13) C  56          s( 10.09%)p 0.57(  5.74%)d 8.34( 84.17%)
1008. (0.00000) RY*(14) C  56          s( 98.48%)p 0.01(  1.11%)d 0.00(  0.41%)
1009. (0.00187) RY*( 1) C  57          s(  1.79%)p46.60( 83.57%)d 8.16( 14.64%)
                                        0.0000  0.0037 -0.0750  0.1108 -0.0023
                                       -0.0034  0.4307  0.0328  0.0064  0.3973
                                        0.0597 -0.0157 -0.6981 -0.0086  0.2045
                                       -0.1301 -0.1375 -0.0012 -0.2621
1010. (0.00134) RY*( 2) C  57          s(  0.12%)p99.99( 86.61%)d99.99( 13.27%)
                                        0.0000  0.0052  0.0301  0.0172 -0.0016
                                        0.0035  0.6855  0.0216 -0.0096 -0.6250
                                       -0.0350  0.0070  0.0505  0.0338  0.0082
                                        0.1834 -0.1517  0.2739  0.0303
1011. (0.00047) RY*( 3) C  57          s( 22.08%)p 3.47( 76.71%)d 0.05(  1.21%)
                                        0.0000 -0.0009 -0.2013  0.4245 -0.0116
                                       -0.0024  0.3393 -0.0366 -0.0114  0.4757
                                        0.1318 -0.0083  0.5976  0.2227  0.0585
                                        0.0394 -0.0709  0.0455  0.0056
1012. (0.00025) RY*( 4) C  57          s( 41.19%)p 1.36( 56.18%)d 0.06(  2.63%)
                                        0.0000 -0.0071  0.5899 -0.2526  0.0019
                                       -0.0011  0.2026 -0.6817  0.0040  0.2245
                                        0.0648  0.0058  0.0345  0.0172 -0.1029
                                        0.0572  0.0557 -0.0050  0.0963
1013. (0.00018) RY*( 5) C  57          s(  4.67%)p14.41( 67.26%)d 6.01( 28.07%)
                                        0.0000 -0.0069  0.1857 -0.1060  0.0304
                                       -0.0059  0.3421  0.3240  0.0074  0.1411
                                       -0.5995  0.0028  0.1484 -0.2218 -0.0482
                                       -0.2562  0.3132 -0.3164  0.1204
1014. (0.00015) RY*( 6) C  57          s( 33.78%)p 1.66( 56.19%)d 0.30( 10.03%)
                                        0.0000 -0.0149 -0.2684  0.5124  0.0549
                                       -0.0024 -0.0594 -0.5564  0.0021 -0.2086
                                       -0.3052  0.0034 -0.0639 -0.3285 -0.1486
                                       -0.2285 -0.0586 -0.1416 -0.0505
1015. (0.00008) RY*( 7) C  57          s( 56.44%)p 0.44( 25.04%)d 0.33( 18.53%)
1016. (0.00006) RY*( 8) C  57          s(  9.60%)p 5.34( 51.26%)d 4.08( 39.14%)
1017. (0.00002) RY*( 9) C  57          s(  2.56%)p 3.63(  9.29%)d34.42( 88.15%)
1018. (0.00003) RY*(10) C  57          s( 18.89%)p 3.92( 74.11%)d 0.37(  7.01%)
1019. (0.00002) RY*(11) C  57          s(  1.89%)p 2.61(  4.94%)d49.20( 93.16%)
1020. (0.00001) RY*(12) C  57          s(  3.87%)p 0.58(  2.26%)d24.25( 93.87%)
1021. (0.00000) RY*(13) C  57          s( 98.43%)p 0.01(  1.19%)d 0.00(  0.38%)
1022. (0.00000) RY*(14) C  57          s(  4.69%)p 1.19(  5.57%)d19.15( 89.74%)
1023. (0.00156) RY*( 1) C  58          s(  7.44%)p 9.86( 73.27%)d 2.59( 19.29%)
                                        0.0000 -0.0066  0.2518 -0.1045 -0.0006
                                       -0.0133 -0.7880 -0.1800  0.0062 -0.0617
                                       -0.1196 -0.0142 -0.2379  0.0652 -0.2421
                                        0.2552 -0.0314 -0.1846  0.1847
1024. (0.00112) RY*( 2) C  58          s(  2.52%)p31.77( 79.92%)d 6.98( 17.57%)
                                        0.0000  0.0027 -0.1095  0.1147  0.0006
                                        0.0012  0.1545  0.0127 -0.0139 -0.5996
                                        0.0977 -0.0075 -0.6365 -0.0260  0.0288
                                       -0.0744  0.1265  0.2222  0.3224
1025. (0.00046) RY*( 3) C  58          s(  4.69%)p20.08( 94.15%)d 0.25(  1.16%)
                                        0.0000  0.0045 -0.0698  0.2049 -0.0001
                                       -0.0087  0.0763  0.0612 -0.0061  0.7031
                                        0.1100  0.0069 -0.6076 -0.2369 -0.0389
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                                    0.0484 -0.0479 -0.0735  0.0041
1026. (0.00018) RY*( 4) C  58      s( 56.89%)p 0.55( 31.50%)d 0.20( 11.61%)
                                    0.0000  0.0050  0.5975 -0.4597 -0.0212
                                   -0.0045  0.2505 -0.1436 -0.0043  0.1651
                                    0.4283 -0.0055 -0.0125  0.1440 -0.0041
                                   -0.0679  0.0376  0.1019  0.3158
1027. (0.00014) RY*( 5) C  58      s( 21.39%)p 2.45( 52.31%)d 1.23( 26.30%)
                                    0.0000  0.0024 -0.2624  0.3805 -0.0160
                                    0.0063 -0.2890 -0.0072 -0.0101  0.1192
                                    0.5553 -0.0044  0.3389 -0.0443  0.0325
                                    0.0487  0.2146  0.2136  0.4098
1028. (0.00010) RY*( 6) C  58      s(  5.13%)p16.39( 84.08%)d 2.10( 10.79%)
1029. (0.00006) RY*( 7) C  58      s(  0.80%)p68.21( 54.71%)d55.46( 44.49%)
1030. (0.00004) RY*( 8) C  58      s(  4.17%)p22.59( 94.12%)d 0.41(  1.71%)
1031. (0.00004) RY*( 9) C  58      s( 82.79%)p 0.09(  7.48%)d 0.12(  9.73%)
1032. (0.00001) RY*(10) C  58      s(  0.99%)p 6.12(  6.05%)d93.94( 92.96%)
1033. (0.00001) RY*(11) C  58      s(  6.56%)p 0.98(  6.45%)d13.26( 86.99%)
1034. (0.00001) RY*(12) C  58      s(  4.82%)p 1.43(  6.91%)d18.33( 88.27%)
1035. (0.00001) RY*(13) C  58      s(  3.27%)p 2.60(  8.50%)d26.98( 88.23%)
1036. (0.00000) RY*(14) C  58      s( 98.56%)p 0.01(  0.73%)d 0.01(  0.71%)
1037. (0.00167) RY*( 1) C  59      s(  5.32%)p14.47( 77.04%)d 3.32( 17.64%)
                                    0.0000 -0.0030  0.1712 -0.1545  0.0057
                                   -0.0044 -0.4947 -0.0820 -0.0042 -0.6189
                                   -0.0630 -0.0170 -0.3566  0.0659 -0.2425
                                    0.0501  0.0381  0.1122  0.3179
1038. (0.00108) RY*( 2) C  59      s(  0.69%)p99.99( 80.45%)d27.28( 18.86%)
                                    0.0000  0.0005  0.0611 -0.0564 -0.0012
                                    0.0085  0.7263 -0.0772 -0.0071 -0.5161
                                    0.0310 -0.0012 -0.0223  0.0555  0.1376
                                   -0.3228  0.1759  0.1608  0.0931
1039. (0.00050) RY*( 3) C  59      s(  5.19%)p17.85( 92.62%)d 0.42(  2.19%)
                                    0.0000  0.0019  0.0192  0.2269 -0.0061
                                   -0.0067  0.2188 -0.1391 -0.0065  0.3363
                                    0.1179  0.0048 -0.8331 -0.1942 -0.0716
                                    0.0030 -0.0191  0.0440  0.1204
1040. (0.00021) RY*( 4) C  59      s( 68.99%)p 0.44( 30.07%)d 0.01(  0.93%)
                                    0.0000 -0.0063  0.7741 -0.3010  0.0065
                                   -0.0008  0.1354 -0.1842  0.0060  0.2799
                                   -0.3540 -0.0079  0.0239  0.2100 -0.0692
                                    0.0362 -0.0508 -0.0221  0.0131
1041. (0.00016) RY*( 5) C  59      s(  1.84%)p44.82( 82.52%)d 8.49( 15.64%)
                                    0.0000  0.0038  0.1287 -0.0376 -0.0205
                                   -0.0045  0.2098  0.7132  0.0051 -0.1774
                                   -0.2749  0.0018 -0.0899 -0.3967 -0.1202
                                    0.3029 -0.1840 -0.1026 -0.0762
1042. (0.00010) RY*( 6) C  59      s( 31.55%)p 1.90( 59.83%)d 0.27(  8.63%)
1043. (0.00008) RY*( 7) C  59      s(  1.58%)p23.38( 36.87%)d39.02( 61.55%)
1044. (0.00005) RY*( 8) C  59      s( 25.17%)p 2.52( 63.53%)d 0.45( 11.30%)
1045. (0.00004) RY*( 9) C  59      s( 50.33%)p 0.78( 39.17%)d 0.21( 10.50%)
1046. (0.00001) RY*(10) C  59      s(  2.65%)p 2.48(  6.59%)d34.20( 90.76%)
1047. (0.00001) RY*(11) C  59      s(  2.49%)p 3.78(  9.40%)d35.44( 88.12%)
1048. (0.00000) RY*(12) C  59      s( 98.99%)p 0.01(  0.74%)d 0.00(  0.27%)
1049. (0.00001) RY*(13) C  59      s(  0.10%)p67.04(  6.51%)d99.99( 93.40%)
1050. (0.00001) RY*(14) C  59      s(  5.11%)p 2.90( 14.84%)d15.65( 80.04%)
1051. (0.00173) RY*( 1) C  60      s(  5.05%)p15.51( 78.28%)d 3.31( 16.68%)
                                    0.0000 -0.0088  0.2127 -0.0718 -0.0011
                                    0.0076 -0.1631 -0.1686 -0.0093 -0.6923
                                   -0.0748  0.0174  0.4893  0.0553 -0.3247
                                    0.2155 -0.0018 -0.0602  0.1062
1052. (0.00133) RY*( 2) C  60      s(  0.23%)p99.99( 87.03%)d55.56( 12.74%)
                                    0.0000  0.0041  0.0466 -0.0103 -0.0002
                                   -0.0024 -0.1142  0.0048  0.0021  0.5711
                                    0.0098  0.0151  0.7269  0.0476  0.1948
                                    0.2499  0.0401 -0.0338  0.1558
1053. (0.00047) RY*( 3) C  60      s( 25.08%)p 2.94( 73.78%)d 0.05(  1.14%)
                                    0.0000  0.0029 -0.3162  0.3883 -0.0061
                                   -0.0144  0.7474  0.2395  0.0044 -0.2047
                                   -0.0910  0.0017  0.2645  0.0376  0.0918
                                    0.0298 -0.0329  0.0228  0.0213
1054. (0.00023) RY*( 4) C  60      s( 54.05%)p 0.70( 37.90%)d 0.15(  8.04%)
                                    0.0000 -0.0064 -0.5018  0.5373  0.0081
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                                     0.0028 -0.5458 -0.0789  0.0101 -0.1548
                                    -0.1355 -0.0012  0.0056 -0.1801  0.2390
                                    -0.0339  0.0287 -0.0766  0.1244
1055. (0.00019) RY*( 5) C  60      s(  9.71%)p 6.48( 62.90%)d 2.82( 27.39%)
                                     0.0000  0.0019  0.2406 -0.1955 -0.0309
                                    -0.0037  0.0441  0.2592  0.0093 -0.0902
                                    -0.5749  0.0078 -0.1546 -0.4441  0.3335
                                     0.3008  0.0801  0.0471  0.2521
1056. (0.00011) RY*( 6) C  60      s(  1.41%)p64.69( 90.91%)d 5.47(  7.68%)
                                     0.0000 -0.0150 -0.0657 -0.0474  0.0852
                                    -0.0033  0.2507 -0.6599 -0.0076  0.1219
                                    -0.1035  0.0057  0.1125 -0.6103 -0.1308
                                    -0.1979  0.0041 -0.1022 -0.1003
1057. (0.00006) RY*( 7) C  60      s( 25.97%)p 1.51( 39.33%)d 1.34( 34.70%)
1058. (0.00003) RY*( 8) C  60      s(  1.92%)p46.22( 88.92%)d 4.76(  9.15%)
1059. (0.00004) RY*( 9) C  60      s( 44.58%)p 0.35( 15.81%)d 0.89( 39.61%)
1060. (0.00001) RY*(10) C  60      s(  8.40%)p 1.21( 10.21%)d 9.68( 81.39%)
1061. (0.00001) RY*(11) C  60      s(  1.23%)p 2.60(  3.20%)d77.64( 95.57%)
1062. (0.00001) RY*(12) C  60      s(  0.10%)p64.51(  6.24%)d99.99( 93.66%)
1063. (0.00001) RY*(13) C  60      s( 24.30%)p 0.18(  4.49%)d 2.93( 71.21%)
1064. (0.00000) RY*(14) C  60      s( 97.96%)p 0.01(  1.20%)d 0.01(  0.84%)
1065. (0.00159) RY*( 1) C  61      s(  8.44%)p 8.68( 73.25%)d 2.17( 18.31%)
                                     0.0000 -0.0069  0.2681 -0.1117 -0.0007
                                     0.0098  0.7183  0.1639 -0.0173 -0.1999
                                     0.1207 -0.0084 -0.3610 -0.0662 -0.2394
                                     0.0838  0.1175 -0.3114  0.0892
1066. (0.00108) RY*( 2) C  61      s(  2.62%)p30.41( 79.83%)d 6.68( 17.54%)
                                     0.0000  0.0026 -0.1109  0.1181  0.0010
                                    -0.0027 -0.3166  0.0107  0.0053  0.0348
                                    -0.0798 -0.0140 -0.8297  0.0417  0.0964
                                     0.1194  0.3403  0.1550  0.1096
1067. (0.00046) RY*( 3) C  61      s(  3.11%)p30.61( 95.27%)d 0.52(  1.62%)
                                     0.0000  0.0050 -0.0588  0.1663 -0.0001
                                     0.0108 -0.1977 -0.0964  0.0084 -0.9291
                                    -0.1933 -0.0012  0.0519 -0.0304 -0.0476
                                    -0.0024 -0.0097 -0.1175 -0.0018
1068. (0.00019) RY*( 4) C  61      s( 44.11%)p 0.88( 38.66%)d 0.39( 17.23%)
                                     0.0000  0.0034  0.5640 -0.3504 -0.0163
                                     0.0025 -0.1936  0.2302 -0.0010 -0.0589
                                    -0.2028 -0.0103  0.1930  0.4628  0.1125
                                     0.1461  0.3398  0.0456  0.1439
1069. (0.00014) RY*( 5) C  61      s( 35.88%)p 1.19( 42.57%)d 0.60( 21.54%)
                                     0.0000 -0.0038 -0.3676  0.4728  0.0123
                                    -0.0069  0.3673 -0.0265  0.0026  0.0457
                                    -0.1719 -0.0091  0.2211  0.4576 -0.0271
                                     0.0224  0.3460  0.1342  0.2766
1070. (0.00010) RY*( 6) C  61      s(  3.50%)p25.63( 89.80%)d 1.91(  6.69%)
1071. (0.00006) RY*( 7) C  61      s(  1.25%)p45.28( 56.44%)d33.94( 42.31%)
1072. (0.00004) RY*( 8) C  61      s(  3.35%)p26.23( 87.89%)d 2.61(  8.76%)
1073. (0.00004) RY*( 9) C  61      s( 79.47%)p 0.10(  8.31%)d 0.15( 12.22%)
1074. (0.00001) RY*(10) C  61      s(  0.55%)p19.49( 10.75%)d99.99( 88.69%)
1075. (0.00001) RY*(11) C  61      s(  1.38%)p 0.99(  1.37%)d70.56( 97.25%)
1076. (0.00001) RY*(12) C  61      s( 16.65%)p 0.70( 11.58%)d 4.31( 71.77%)
1077. (0.00000) RY*(13) C  61      s( 98.85%)p 0.01(  0.94%)d 0.00(  0.21%)
1078. (0.00001) RY*(14) C  61      s(  0.83%)p 4.24(  3.51%)d99.99( 95.67%)
1079. (0.00178) RY*( 1) C  62      s(  3.90%)p20.59( 80.33%)d 4.04( 15.76%)
                                     0.0000 -0.0012  0.1410 -0.1382  0.0042
                                     0.0025  0.4603  0.0253  0.0147  0.7545
                                     0.0758  0.0126  0.1060 -0.0642 -0.1967
                                     0.1369  0.2611 -0.0385  0.1748
1080. (0.00127) RY*( 2) C  62      s(  1.27%)p67.26( 85.19%)d10.69( 13.54%)
                                     0.0000  0.0038 -0.0232  0.1099 -0.0051
                                    -0.0041 -0.7585  0.0517  0.0089  0.5086
                                     0.0361 -0.0029 -0.0873  0.0782 -0.0590
                                    -0.2530  0.1880  0.0637 -0.1690
1081. (0.00040) RY*( 3) C  62      s( 23.33%)p 3.27( 76.26%)d 0.02(  0.41%)
                                     0.0000  0.0020 -0.3315  0.3510 -0.0155
                                     0.0031 -0.0083 -0.1771  0.0008  0.0321
                                     0.1373 -0.0156  0.8009  0.2638  0.0398
                                     0.0145 -0.0051 -0.0185  0.0438
1082. (0.00023) RY*( 4) C  62      s( 32.53%)p 2.00( 64.96%)d 0.08(  2.52%)
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                                        0.0000 -0.0015  0.5613 -0.0999 -0.0140
                                       -0.0020 -0.0997  0.6255 -0.0001 -0.1671
                                       -0.1659  0.0022  0.3716  0.2341 -0.0723
                                       -0.0369  0.1124 -0.0420  0.0648
1083. (0.00016) RY*( 5) C  62        s(  4.09%)p16.33( 66.81%)d 7.11( 29.10%)
                                        0.0000 -0.0144  0.1954  0.0197  0.0462
                                        0.0079 -0.3246  0.0229 -0.0058  0.0239
                                        0.2666  0.0053  0.2184 -0.6654  0.1223
                                        0.4110 -0.2164 -0.0395  0.2425
1084. (0.00012) RY*( 6) C  62        s( 37.10%)p 1.48( 54.73%)d 0.22(  8.18%)
                                        0.0000 -0.0122 -0.4030  0.4543  0.0444
                                        0.0011  0.1584  0.6149  0.0048  0.0862
                                       -0.2110 -0.0022 -0.0871 -0.2908 -0.0455
                                        0.0954 -0.0362 -0.0870 -0.2485
1085. (0.00007) RY*( 7) C  62        s( 63.93%)p 0.43( 27.33%)d 0.14(  8.75%)
1086. (0.00007) RY*( 8) C  62        s(  5.40%)p10.02( 54.08%)d 7.51( 40.52%)
1087. (0.00003) RY*( 9) C  62        s(  1.38%)p 8.83( 12.22%)d62.40( 86.40%)
1088. (0.00004) RY*(10) C  62        s( 14.48%)p 4.55( 65.86%)d 1.36( 19.66%)
1089. (0.00000) RY*(11) C  62        s( 98.76%)p 0.01(  1.17%)d 0.00(  0.07%)
1090. (0.00001) RY*(12) C  62        s(  1.46%)p 2.44(  3.57%)d64.88( 94.97%)
1091. (0.00001) RY*(13) C  62        s(  6.41%)p 0.22(  1.38%)d14.39( 92.21%)
1092. (0.00001) RY*(14) C  62        s(  5.97%)p 1.06(  6.30%)d14.70( 87.73%)
1093. (0.00043) RY*( 1) H  63        s( 99.24%)p 0.01(  0.76%)
                                       -0.0010  0.9961  0.0108 -0.0448  0.0676
                                        0.0317
1094. (0.00028) RY*( 2) H  63        s(  3.98%)p24.14( 96.02%)
                                        0.0002 -0.0799  0.1828 -0.2234  0.6891
                                        0.6599
1095. (0.00011) RY*( 3) H  63        s(  0.09%)p99.99( 99.91%)
                                       -0.0014  0.0244 -0.0171  0.0234 -0.6833
                                        0.7291
1096. (0.00010) RY*( 4) H  63        s( 82.23%)p 0.22( 17.77%)
1097. (0.00003) RY*( 5) H  63        s( 14.52%)p 5.88( 85.48%)
1098. (0.00043) RY*( 1) H  64        s( 98.90%)p 0.01(  1.10%)
                                       -0.0008  0.9945  0.0069  0.0413  0.0260
                                        0.0928
1099. (0.00028) RY*( 2) H  64        s(  1.51%)p65.32( 98.49%)
                                        0.0001 -0.0707  0.1004 -0.2399  0.7009
                                        0.6603
1100. (0.00011) RY*( 3) H  64        s(  2.34%)p41.66( 97.66%)
                                        0.0000  0.0646  0.1388 -0.9505 -0.1030
                                       -0.2501
1101. (0.00010) RY*( 4) H  64        s( 85.22%)p 0.17( 14.78%)
                                        0.0089 -0.0232  0.9228  0.1092 -0.2995
                                        0.2148
1102. (0.00003) RY*( 5) H  64        s( 12.09%)p 7.27( 87.91%)
1103. (0.00120) RY*( 1) H  65        s( 99.17%)p 0.01(  0.83%)
                                       -0.0032  0.9958  0.0055  0.0033 -0.0316
                                       -0.0851
1104. (0.00029) RY*( 2) H  65        s( 26.01%)p 2.85( 73.99%)
                                       -0.0007 -0.0115  0.5098 -0.7527 -0.4158
                                        0.0240
1105. (0.00026) RY*( 3) H  65        s( 64.44%)p 0.55( 35.56%)
                                        0.0000 -0.0233  0.8024  0.3361  0.3566
                                       -0.3398
1106. (0.00011) RY*( 4) H  65        s( 10.00%)p 9.00( 90.00%)
                                       -0.0018  0.0652  0.3094  0.3394 -0.1867
                                        0.8660
1107. (0.00004) RY*( 5) H  65        s(  0.43%)p99.99( 99.57%)
1108. (0.00029) RY*( 1) H  66        s( 99.82%)p 0.00(  0.18%)
                                       -0.0019  0.9991  0.0059  0.0340  0.0150
                                        0.0208
1109. (0.00022) RY*( 2) H  66        s(  0.13%)p99.99( 99.87%)
                                        0.0000  0.0340  0.0122 -0.8391 -0.5298
                                        0.1179
1110. (0.00018) RY*( 3) H  66        s( 99.72%)p 0.00(  0.28%)
                                       -0.0012 -0.0076  0.9985  0.0132  0.0127
                                        0.0501
1111. (0.00012) RY*( 4) H  66        s(  0.19%)p99.99( 99.81%)
                                        0.0003  0.0145  0.0408  0.2887 -0.6179
                                       -0.7301
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1112. (0.00002) RY*( 5) H  66          s(  0.20%)p99.99( 99.80%)
1113. (0.00103) RY*( 1) H  67          s( 98.65%)p 0.01(  1.35%)
                                        0.0032  0.9932 -0.0069  0.0064 -0.1096
                                       -0.0375
1114. (0.00028) RY*( 2) H  67          s( 84.68%)p 0.18( 15.32%)
                                       -0.0008  0.0269  0.9198 -0.3262  0.1972
                                       -0.0886
1115. (0.00024) RY*( 3) H  67          s(  4.23%)p22.63( 95.77%)
                                        0.0016  0.0380  0.2022  0.8692  0.4288
                                       -0.1354
1116. (0.00013) RY*( 4) H  67          s( 11.87%)p 7.43( 88.13%)
                                       -0.0003 -0.0837  0.3341  0.3715 -0.8333
                                        0.2211
1117. (0.00004) RY*( 5) H  67          s(  0.62%)p99.99( 99.38%)
1118. (0.00136) RY*( 1) H  68          s( 99.24%)p 0.01(  0.76%)
                                        0.0031  0.9962 -0.0038 -0.0083 -0.0608
                                       -0.0619
1119. (0.00033) RY*( 2) H  68          s( 60.61%)p 0.65( 39.39%)
                                       -0.0010  0.0021  0.7785 -0.2316 -0.4077
                                        0.4172
1120. (0.00025) RY*( 3) H  68          s( 31.85%)p 2.14( 68.15%)
                                        0.0008  0.0289  0.5636  0.5856  0.5504
                                       -0.1890
1121. (0.00011) RY*( 4) H  68          s(  7.86%)p11.72( 92.14%)
                                       -0.0014 -0.0581  0.2743 -0.4752 -0.0580
                                       -0.8320
1122. (0.00004) RY*( 5) H  68          s(  0.49%)p99.99( 99.51%)
1123. (0.00031) RY*( 1) H  69          s( 98.47%)p 0.02(  1.53%)
                                       -0.0022  0.9922 -0.0151  0.0465  0.0774
                                       -0.0845
1124. (0.00024) RY*( 2) H  69          s( 13.29%)p 6.53( 86.71%)
                                       -0.0002  0.1174  0.3451 -0.5237 -0.6091
                                        0.4710
1125. (0.00018) RY*( 3) H  69          s( 87.95%)p 0.14( 12.05%)
                                       -0.0007 -0.0270  0.9374  0.1739  0.2605
                                       -0.1498
1126. (0.00012) RY*( 4) H  69          s(  0.20%)p99.99( 99.80%)
                                       -0.0003 -0.0108  0.0437  0.2951 -0.7176
                                       -0.6293
1127. (0.00002) RY*( 5) H  69          s(  0.15%)p99.99( 99.85%)
1128. (0.00114) RY*( 1) H  70          s( 99.17%)p 0.01(  0.83%)
                                       -0.0031  0.9958  0.0057  0.0680 -0.0438
                                       -0.0417
1129. (0.00027) RY*( 2) H  70          s( 89.04%)p 0.12( 10.96%)
                                       -0.0006 -0.0279  0.9432  0.2883 -0.1416
                                        0.0802
1130. (0.00026) RY*( 3) H  70          s(  0.42%)p99.99( 99.58%)
                                       -0.0002  0.0313  0.0570 -0.6226 -0.6525
                                        0.4270
1131. (0.00011) RY*( 4) H  70          s( 11.05%)p 8.05( 88.95%)
                                       -0.0017  0.0592  0.3271 -0.7227  0.5357
                                       -0.2832
1132. (0.00004) RY*( 5) H  70          s(  0.37%)p99.99( 99.63%)
1133. (0.00044) RY*( 1) H  71          s( 99.83%)p 0.00(  0.17%)
                                       -0.0010  0.9991  0.0056  0.0364 -0.0179
                                        0.0070
1134. (0.00033) RY*( 2) H  71          s(  2.67%)p36.40( 97.33%)
                                        0.0001 -0.0256  0.1615  0.4321 -0.1546
                                        0.8733
1135. (0.00012) RY*( 3) H  71          s(  0.25%)p99.99( 99.75%)
                                        0.0019 -0.0131  0.0483 -0.1072 -0.9844
                                       -0.1306
1136. (0.00010) RY*( 4) H  71          s( 84.66%)p 0.18( 15.34%)
1137. (0.00003) RY*( 5) H  71          s( 12.65%)p 6.91( 87.35%)
1138. (0.00044) RY*( 1) H  72          s( 99.55%)p 0.00(  0.45%)
                                       -0.0010  0.9977  0.0107  0.0165  0.0270
                                        0.0591
1139. (0.00033) RY*( 2) H  72          s(  4.21%)p22.73( 95.79%)
                                        0.0001 -0.0570  0.1972  0.4318 -0.1354
                                        0.8678
1140. (0.00011) RY*( 3) H  72          s(  1.80%)p54.61( 98.20%)
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                                      0.0020 -0.0216  0.1323 -0.8356  0.3106
                                      0.4327
1141. (0.00010) RY*( 4) H  72       s( 84.30%)p 0.19( 15.70%)
                                      0.0079 -0.0063  0.9181  0.1350  0.2927
                                     -0.2306
1142. (0.00003) RY*( 5) H  72       s( 10.21%)p 8.80( 89.79%)
1143. (0.00131) RY*( 1) H  73       s( 99.22%)p 0.01(  0.78%)
                                     -0.0034  0.9961  0.0050 -0.0290 -0.0362
                                     -0.0754
1144. (0.00028) RY*( 2) H  73       s( 45.54%)p 1.20( 54.46%)
                                     -0.0009 -0.0136  0.6747  0.5761  0.1594
                                     -0.4328
1145. (0.00026) RY*( 3) H  73       s( 46.18%)p 1.17( 53.82%)
                                     -0.0002 -0.0218  0.6792 -0.5211 -0.4806
                                      0.1888
1146. (0.00011) RY*( 4) H  73       s(  8.78%)p10.39( 91.22%)
                                     -0.0021  0.0655  0.2889 -0.1202  0.7586
                                      0.5677
1147. (0.00004) RY*( 5) H  73       s(  0.34%)p99.99( 99.66%)
1148. (0.00032) RY*( 1) H  74       s( 99.63%)p 0.00(  0.37%)
                                     -0.0019  0.9981  0.0042  0.0394  0.0410
                                     -0.0214
1149. (0.00023) RY*( 2) H  74       s(  0.59%)p99.99( 99.41%)
                                     -0.0006  0.0574  0.0507 -0.7912 -0.4061
                                      0.4509
1150. (0.00019) RY*( 3) H  74       s( 99.54%)p 0.00(  0.46%)
                                     -0.0009 -0.0075  0.9977  0.0547  0.0365
                                      0.0177
1151. (0.00012) RY*( 4) H  74       s(  0.18%)p99.99( 99.82%)
                                      0.0003  0.0002  0.0420 -0.5009  0.0216
                                     -0.8642
1152. (0.00002) RY*( 5) H  74       s(  0.12%)p99.99( 99.88%)
1153. (0.00114) RY*( 1) H  75       s( 98.84%)p 0.01(  1.16%)
                                      0.0036  0.9942 -0.0061 -0.0378  0.0516
                                     -0.0865
1154. (0.00028) RY*( 2) H  75       s( 91.45%)p 0.09(  8.55%)
                                     -0.0008  0.0293  0.9559  0.1130 -0.2621
                                      0.0637
1155. (0.00024) RY*( 3) H  75       s(  0.03%)p99.99( 99.97%)
                                      0.0015  0.0158 -0.0085 -0.8717 -0.3136
                                      0.3762
1156. (0.00014) RY*( 4) H  75       s(  9.20%)p 9.87( 90.80%)
                                      0.0000 -0.0803  0.2925 -0.4162  0.8106
                                     -0.2787
1157. (0.00004) RY*( 5) H  75       s(  0.53%)p99.99( 99.47%)
1158. (0.00129) RY*( 1) H  76       s( 98.63%)p 0.01(  1.37%)
                                      0.0036  0.9931 -0.0039 -0.0033  0.0438
                                     -0.1087
1159. (0.00032) RY*( 2) H  76       s( 68.04%)p 0.47( 31.96%)
                                     -0.0012 -0.0030  0.8249  0.1841  0.5144
                                      0.1450
1160. (0.00024) RY*( 3) H  76       s( 21.80%)p 3.59( 78.20%)
                                      0.0009  0.0579  0.4633 -0.5662 -0.6189
                                      0.2801
1161. (0.00013) RY*( 4) H  76       s( 10.88%)p 8.19( 89.12%)
                                     -0.0004 -0.0715  0.3220  0.2612 -0.3778
                                     -0.8247
1162. (0.00004) RY*( 5) H  76       s(  0.70%)p99.99( 99.30%)
1163. (0.00031) RY*( 1) H  77       s( 99.66%)p 0.00(  0.34%)
                                     -0.0021  0.9983  0.0051  0.0395  0.0257
                                     -0.0350
1164. (0.00022) RY*( 2) H  77       s(  0.32%)p99.99( 99.68%)
                                      0.0001  0.0513  0.0234 -0.5970 -0.7668
                                      0.2289
1165. (0.00019) RY*( 3) H  77       s( 99.19%)p 0.01(  0.81%)
                                     -0.0012 -0.0061  0.9959  0.0758 -0.0156
                                      0.0454
1166. (0.00012) RY*( 4) H  77       s(  0.68%)p99.99( 99.32%)
                                     -0.0001 -0.0122  0.0813 -0.5433  0.1812
                                     -0.8156
1167. (0.00002) RY*( 5) H  77       s(  0.21%)p99.99( 99.79%)
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1168. (0.00125) RY*( 1) H  78          s( 99.21%)p 0.01(  0.79%)
                                        -0.0033  0.9960  0.0052 -0.0757  0.0264
                                        -0.0378
1169. (0.00026) RY*( 2) H  78          s( 89.99%)p 0.11( 10.01%)
                                        -0.0005 -0.0269  0.9482 -0.2481  0.1894
                                         0.0517
1170. (0.00026) RY*( 3) H  78          s(  0.03%)p99.99( 99.97%)
                                         0.0000  0.0133  0.0124  0.5779  0.7702
                                        -0.2691
1171. (0.00011) RY*( 4) H  78          s( 10.48%)p 8.55( 89.52%)
                                        -0.0022  0.0642  0.3172  0.7240 -0.5950
                                        -0.1304
1172. (0.00004) RY*( 5) H  78          s(  0.34%)p99.99( 99.66%)
1173. (0.00168) RY*( 1) H  79          s( 99.90%)p 0.00(  0.10%)
                                        -0.0058  0.9995  0.0002 -0.0097 -0.0266
                                        -0.0154
1174. (0.00027) RY*( 2) H  79          s( 30.00%)p 2.33( 70.00%)
                                        -0.0057  0.0120  0.5475  0.3758 -0.1087
                                         0.7396
1175. (0.00017) RY*( 3) H  79          s(  3.51%)p27.51( 96.49%)
                                        -0.0013  0.0109  0.1870  0.7648  0.4009
                                        -0.4683
1176. (0.00013) RY*( 4) H  79          s( 58.21%)p 0.72( 41.79%)
                                        -0.0034 -0.0193  0.7627 -0.2930 -0.3398
                                        -0.4654
1177. (0.00001) RY*( 5) H  79          s(  8.44%)p10.85( 91.56%)
1178. (0.00357) RY*( 1) H  80          s( 99.94%)p 0.00(  0.06%)
                                         0.0068  0.9997 -0.0013  0.0041  0.0216
                                        -0.0102
1179. (0.00027) RY*( 2) H  80          s( 84.48%)p 0.18( 15.52%)
                                        -0.0074 -0.0032  0.9191  0.3599  0.0684
                                        -0.1449
1180. (0.00017) RY*( 3) H  80          s(  6.35%)p14.76( 93.65%)
                                         0.0028  0.0073  0.2518 -0.7524 -0.3984
                                        -0.4601
1181. (0.00013) RY*( 4) H  80          s(  3.42%)p28.25( 96.58%)
                                         0.0006  0.0219  0.1836 -0.0483 -0.6459
                                         0.7392
1182. (0.00002) RY*( 5) H  80          s(  5.86%)p16.05( 94.14%)
1183. (0.00179) RY*( 1) H  81          s( 99.68%)p 0.00(  0.32%)
                                        -0.0058  0.9984 -0.0006 -0.0562 -0.0053
                                         0.0022
1184. (0.00029) RY*( 2) H  81          s( 31.82%)p 2.14( 68.18%)
                                        -0.0055  0.0267  0.5634  0.4970 -0.0385
                                         0.6583
1185. (0.00019) RY*( 3) H  81          s(  9.39%)p 9.65( 90.61%)
                                         0.0001  0.0214  0.3057  0.2838  0.8004
                                        -0.4300
1186. (0.00013) RY*( 4) H  81          s( 51.83%)p 0.93( 48.17%)
                                        -0.0038 -0.0382  0.7189 -0.6802 -0.0890
                                        -0.1054
1187. (0.00002) RY*( 5) H  81          s(  7.33%)p12.65( 92.67%)
1188. (0.00302) RY*( 1) H  82          s( 99.90%)p 0.00(  0.10%)
                                         0.0064  0.9995 -0.0011  0.0233  0.0042
                                        -0.0200
1189. (0.00024) RY*( 2) H  82          s( 82.32%)p 0.21( 17.68%)
                                        -0.0059 -0.0074  0.9072  0.1263  0.3484
                                        -0.1987
1190. (0.00018) RY*( 3) H  82          s(  0.79%)p99.99( 99.21%)
                                         0.0027  0.0111  0.0882 -0.8489 -0.1969
                                        -0.4824
1191. (0.00013) RY*( 4) H  82          s( 12.93%)p 6.73( 87.07%)
                                         0.0004  0.0255  0.3587 -0.3303 -0.3607
                                         0.7946
1192. (0.00002) RY*( 5) H  82          s(  4.10%)p23.38( 95.90%)
1193. (0.00174) RY*( 1) H  83          s( 99.82%)p 0.00(  0.18%)
                                        -0.0057  0.9991  0.0000  0.0231  0.0234
                                        -0.0264
1194. (0.00026) RY*( 2) H  83          s( 25.74%)p 2.88( 74.26%)
                                        -0.0048  0.0106  0.5072 -0.2993  0.5299
                                         0.6101
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1195. (0.00018) RY*( 3) H  83           s(  2.50%)p39.02( 97.50%)
                                         -0.0005  0.0322  0.1548 -0.7895 -0.5931
                                         -0.0015
1196. (0.00012) RY*( 4) H  83           s( 64.71%)p 0.55( 35.29%)
                                         -0.0037 -0.0186  0.8042  0.1716 -0.0181
                                         -0.5684
1197. (0.00002) RY*( 5) H  83           s(  7.27%)p12.76( 92.73%)
1198. (0.00176) RY*( 1) H  84           s( 99.97%)p 0.00(  0.03%)
                                         -0.0053  0.9998  0.0019 -0.0063  0.0132
                                         -0.0082
1199. (0.00023) RY*( 2) H  84           s( 66.89%)p 0.49( 33.11%)
                                         -0.0042 -0.0015  0.8179  0.1182 -0.2579
                                         -0.5006
1200. (0.00017) RY*( 3) H  84           s(  3.50%)p27.55( 96.50%)
                                         -0.0038  0.0072  0.1870 -0.6381 -0.5896
                                          0.4585
1201. (0.00013) RY*( 4) H  84           s( 25.88%)p 2.86( 74.12%)
                                         -0.0009 -0.0087  0.5086 -0.2312  0.7248
                                          0.4030
1202. (0.00002) RY*( 5) H  84           s(  3.80%)p25.31( 96.20%)
1203. (0.00183) RY*( 1) H  85           s( 99.55%)p 0.00(  0.45%)
                                         -0.0059  0.9977 -0.0012  0.0548  0.0211
                                         -0.0318
1204. (0.00029) RY*( 2) H  85           s( 32.77%)p 2.05( 67.23%)
                                         -0.0049  0.0322  0.5715 -0.3274  0.3542
                                          0.6631
1205. (0.00018) RY*( 3) H  85           s(  4.70%)p20.27( 95.30%)
                                          0.0009  0.0374  0.2136 -0.1901 -0.9323
                                          0.2183
1206. (0.00012) RY*( 4) H  85           s( 55.23%)p 0.81( 44.77%)
                                         -0.0044 -0.0410  0.7420  0.5771 -0.0283
                                         -0.3375
1207. (0.00002) RY*( 5) H  85           s(  7.79%)p11.83( 92.21%)
1208. (0.00160) RY*( 1) H  86           s( 99.75%)p 0.00(  0.25%)
                                         -0.0051  0.9987 -0.0007  0.0236  0.0435
                                          0.0061
1209. (0.00025) RY*( 2) H  86           s( 30.18%)p 2.31( 69.82%)
                                         -0.0048  0.0253  0.5488  0.2406 -0.6357
                                         -0.4859
1210. (0.00017) RY*( 3) H  86           s(  5.84%)p16.12( 94.16%)
                                         -0.0013  0.0314  0.2396 -0.6010 -0.4748
                                          0.5958
1211. (0.00012) RY*( 4) H  86           s( 59.66%)p 0.68( 40.34%)
                                         -0.0022 -0.0286  0.7719  0.2176  0.5070
                                          0.3146
1212. (0.00002) RY*( 5) H  86           s(  4.61%)p20.67( 95.39%)
1213. (0.00064) RY*( 1) H  87           s( 91.51%)p 0.09(  8.49%)
                                         -0.0009  0.9566 -0.0058  0.0139 -0.0305
                                          0.2894
1214. (0.00019) RY*( 2) H  87           s( 17.32%)p 4.77( 82.68%)
                                         -0.0010  0.1027  0.4033 -0.7588 -0.3730
                                         -0.3344
1215. (0.00012) RY*( 3) H  87           s( 83.41%)p 0.20( 16.59%)
                                         -0.0012 -0.0305  0.9128  0.3132  0.2267
                                          0.1279
1216. (0.00007) RY*( 4) H  87           s(  7.42%)p12.47( 92.58%)
1217. (0.00002) RY*( 5) H  87           s(  0.37%)p99.99( 99.63%)
1218. (0.00071) RY*( 1) H  88           s( 95.32%)p 0.05(  4.68%)
                                         -0.0016  0.9760 -0.0241 -0.1651  0.0238
                                          0.1378
1219. (0.00024) RY*( 2) H  88           s( 58.04%)p 0.72( 41.96%)
                                         -0.0028  0.1094  0.7540  0.2900 -0.5430
                                         -0.2017
1220. (0.00012) RY*( 3) H  88           s( 24.37%)p 3.10( 75.63%)
                                         -0.0007  0.0408  0.4920  0.2048  0.8389
                                         -0.1027
1221. (0.00007) RY*( 4) H  88           s( 17.70%)p 4.65( 82.30%)
1222. (0.00002) RY*( 5) H  88           s(  4.62%)p20.66( 95.38%)
1223. (0.00090) RY*( 1) H  89           s( 98.67%)p 0.01(  1.33%)
                                         -0.0026  0.9933 -0.0049 -0.0244 -0.0309
                                          0.1085
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1224. (0.00019) RY*( 2) H  89          s( 74.40%)p 0.34( 25.60%)
                                        -0.0053  0.0520  0.8610 -0.0846 -0.1077
                                        -0.4871
1225. (0.00012) RY*( 3) H  89          s(  0.09%)p99.99( 99.91%)
                                         0.0002 -0.0017  0.0297  0.8177 -0.5737
                                         0.0372
1226. (0.00010) RY*( 4) H  89          s( 26.41%)p 2.79( 73.59%)
                                         0.0089 -0.0784  0.5078  0.0963  0.2173
                                         0.8243
1227. (0.00002) RY*( 5) H  89          s(  0.49%)p99.99( 99.51%)
1228. (0.00064) RY*( 1) H  90          s( 92.43%)p 0.08(  7.57%)
                                        -0.0006  0.9614 -0.0088  0.2516  0.1095
                                         0.0199
1229. (0.00016) RY*( 2) H  90          s( 33.79%)p 1.96( 66.21%)
                                        -0.0008  0.0073  0.5812  0.0341 -0.2372
                                         0.7776
1230. (0.00013) RY*( 3) H  90          s( 60.83%)p 0.64( 39.17%)
                                        -0.0018  0.0879  0.7750 -0.3043  0.0884
                                        -0.5397
1231. (0.00006) RY*( 4) H  90          s( 11.79%)p 7.48( 88.21%)
1232. (0.00002) RY*( 5) H  90          s(  1.21%)p81.84( 98.79%)
1233. (0.00062) RY*( 1) H  91          s( 95.41%)p 0.05(  4.59%)
                                        -0.0023  0.9766 -0.0203  0.1540  0.1478
                                         0.0177
1234. (0.00015) RY*( 2) H  91          s( 50.53%)p 0.98( 49.47%)
                                        -0.0034  0.1168  0.7012  0.0188 -0.6697
                                        -0.2142
1235. (0.00015) RY*( 3) H  91          s(  7.30%)p12.69( 92.70%)
                                        -0.0024  0.0859  0.2562 -0.8245  0.3673
                                        -0.3351
1236. (0.00004) RY*( 4) H  91          s( 45.83%)p 1.18( 54.17%)
1237. (0.00002) RY*( 5) H  91          s(  0.97%)p99.99( 99.03%)
1238. (0.00089) RY*( 1) H  92          s( 96.20%)p 0.04(  3.80%)
                                        -0.0020  0.9808 -0.0047  0.0692  0.1794
                                        -0.0315
1239. (0.00014) RY*( 2) H  92          s(  2.94%)p33.01( 97.06%)
                                         0.0001 -0.0023  0.1715 -0.5622  0.3611
                                         0.7240
1240. (0.00013) RY*( 3) H  92          s( 88.54%)p 0.13( 11.46%)
                                        -0.0018  0.0632  0.9388  0.0191 -0.3356
                                        -0.0399
1241. (0.00006) RY*( 4) H  92          s( 11.97%)p 7.35( 88.03%)
1242. (0.00002) RY*( 5) H  92          s(  0.39%)p99.99( 99.61%)
1243. (0.00063) RY*( 1) H  93          s( 91.63%)p 0.09(  8.37%)
                                        -0.0003  0.9572 -0.0086  0.2856 -0.0328
                                         0.0326
1244. (0.00014) RY*( 2) H  93          s( 96.00%)p 0.04(  4.00%)
                                        -0.0027  0.0627  0.9778 -0.1731 -0.0300
                                        -0.0954
1245. (0.00014) RY*( 3) H  93          s(  0.12%)p99.99( 99.88%)
                                        -0.0013  0.0347  0.0026  0.0275  0.9528
                                        -0.3004
1246. (0.00006) RY*( 4) H  93          s( 10.34%)p 8.67( 89.66%)
1247. (0.00002) RY*( 5) H  93          s(  1.95%)p50.25( 98.05%)
1248. (0.00076) RY*( 1) H  94          s( 95.94%)p 0.04(  4.06%)
                                        -0.0022  0.9794 -0.0143  0.1662  0.0378
                                        -0.1073
1249. (0.00018) RY*( 2) H  94          s( 64.52%)p 0.55( 35.48%)
                                        -0.0011  0.0946  0.7976 -0.1989  0.2070
                                         0.5219
1250. (0.00015) RY*( 3) H  94          s( 16.60%)p 5.02( 83.40%)
                                        -0.0007  0.0389  0.4056 -0.3590 -0.6787
                                        -0.4945
1251. (0.00006) RY*( 4) H  94          s( 22.89%)p 3.37( 77.11%)
1252. (0.00002) RY*( 5) H  94          s(  0.10%)p99.99( 99.90%)
1253. (0.00054) RY*( 1) H  95          s( 92.95%)p 0.08(  7.05%)
                                        -0.0017  0.9640 -0.0138  0.2287 -0.0720
                                        -0.1142
1254. (0.00014) RY*( 2) H  95          s( 10.59%)p 8.44( 89.41%)
                                        -0.0006  0.0474  0.3219  0.2063 -0.2004
                                         0.9008
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1255. (0.00013) RY*( 3) H  95          s( 74.08%)p 0.35( 25.92%)
                                        -0.0015  0.1075  0.8540 -0.3904  0.2860
                                        -0.1578
1256. (0.00007) RY*( 4) H  95          s( 21.71%)p 3.61( 78.29%)
1257. (0.00001) RY*( 5) H  95          s(  0.71%)p99.99( 99.29%)
1258. (0.00077) RY*( 1) H  96          s( 95.89%)p 0.04(  4.11%)
                                        -0.0006  0.9792  0.0039 -0.0262 -0.1883
                                         0.0705
1259. (0.00018) RY*( 2) H  96          s( 47.67%)p 1.10( 52.33%)
                                        -0.0020 -0.0189  0.6902 -0.7140 -0.0268
                                        -0.1130
1260. (0.00013) RY*( 3) H  96          s( 46.22%)p 1.16( 53.78%)
                                        -0.0004 -0.0519  0.6779  0.6564 -0.3178
                                         0.0770
1261. (0.00010) RY*( 4) H  96          s(  9.42%)p 9.62( 90.58%)
1262. (0.00002) RY*( 5) H  96          s(  0.85%)p99.99( 99.15%)
1263. (0.00090) RY*( 1) H  97          s( 97.95%)p 0.02(  2.05%)
                                        -0.0017  0.9897  0.0003 -0.0402 -0.1299
                                        -0.0452
1264. (0.00025) RY*( 2) H  97          s( 93.72%)p 0.07(  6.28%)
                                        -0.0021  0.0029  0.9681 -0.0092 -0.0579
                                         0.2436
1265. (0.00012) RY*( 3) H  97          s(  5.67%)p16.62( 94.33%)
                                        -0.0001 -0.0075  0.2381 -0.2547  0.3280
                                        -0.8779
1266. (0.00009) RY*( 4) H  97          s(  2.05%)p47.83( 97.95%)
1267. (0.00002) RY*( 5) H  97          s(  0.65%)p99.99( 99.35%)
1268. (0.00071) RY*( 1) H  98          s( 95.86%)p 0.04(  4.14%)
                                        -0.0024  0.9790 -0.0103 -0.0960 -0.1580
                                        -0.0851
1269. (0.00020) RY*( 2) H  98          s( 64.17%)p 0.56( 35.83%)
                                        -0.0021  0.0545  0.7992 -0.2255  0.1325
                                         0.5384
1270. (0.00014) RY*( 3) H  98          s( 15.30%)p 5.54( 84.70%)
                                         0.0003  0.1095  0.3755  0.7837  0.3544
                                        -0.3274
1271. (0.00009) RY*( 4) H  98          s( 24.55%)p 3.07( 75.45%)
1272. (0.00002) RY*( 5) H  98          s(  0.17%)p99.99( 99.83%)
1273. (0.00062) RY*( 1) H  99          s( 91.51%)p 0.09(  8.49%)
                                        -0.0004  0.9566 -0.0093 -0.0206  0.2420
                                        -0.1610
1274. (0.00014) RY*( 2) H  99          s( 95.87%)p 0.04(  4.13%)
                                        -0.0026  0.0661  0.9769 -0.0028 -0.1107
                                         0.1703
1275. (0.00014) RY*( 3) H  99          s(  0.20%)p99.99( 99.80%)
                                        -0.0012  0.0439 -0.0075  0.9928 -0.1080
                                        -0.0278
1276. (0.00006) RY*( 4) H  99          s( 10.57%)p 8.46( 89.43%)
1277. (0.00002) RY*( 5) H  99          s(  1.89%)p51.93( 98.11%)
1278. (0.00080) RY*( 1) H 100          s( 95.86%)p 0.04(  4.14%)
                                        -0.0021  0.9790 -0.0112  0.0950  0.1799
                                         0.0038
1279. (0.00016) RY*( 2) H 100          s( 82.73%)p 0.21( 17.27%)
                                        -0.0009  0.0947  0.9046 -0.1583 -0.3736
                                        -0.0900
1280. (0.00015) RY*( 3) H 100          s(  0.89%)p99.99( 99.11%)
                                        -0.0006  0.0024  0.0943 -0.4594  0.2174
                                         0.8560
1281. (0.00006) RY*( 4) H 100          s( 20.39%)p 3.91( 79.61%)
1282. (0.00002) RY*( 5) H 100          s(  0.18%)p99.99( 99.82%)
1283. (0.00056) RY*( 1) H 101          s( 93.59%)p 0.07(  6.41%)
                                        -0.0016  0.9673 -0.0128 -0.0117  0.2526
                                        -0.0121
1284. (0.00013) RY*( 2) H 101          s( 86.27%)p 0.16( 13.73%)
                                        -0.0018  0.1054  0.9228  0.0874 -0.3555
                                        -0.0577
1285. (0.00014) RY*( 3) H 101          s(  0.02%)p99.99( 99.98%)
                                         0.0000  0.0118  0.0061  0.5535  0.0204
                                         0.8325
1286. (0.00007) RY*( 4) H 101          s( 19.46%)p 4.14( 80.54%)
1287. (0.00001) RY*( 5) H 101          s(  0.70%)p99.99( 99.30%)
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1288. (0.00060) RY*( 1) H 102           s( 92.64%)p 0.08(  7.36%)
                                         -0.0006  0.9624  0.0099 -0.2689  0.0145
                                          0.0336
1289. (0.00018) RY*( 2) H 102           s( 53.59%)p 0.87( 46.41%)
                                         -0.0014 -0.0447  0.7307 -0.1109 -0.5346
                                          0.4074
1290. (0.00013) RY*( 3) H 102           s( 34.11%)p 1.93( 65.89%)
                                          0.0013 -0.1161  0.5724 -0.4029  0.6191
                                         -0.3366
1291. (0.00010) RY*( 4) H 102           s( 19.32%)p 4.18( 80.68%)
                                         -0.0035  0.2407  0.3678  0.8651  0.1810
                                         -0.1602
1292. (0.00002) RY*( 5) H 102           s(  0.38%)p99.99( 99.62%)
1293. (0.00071) RY*( 1) H 103           s( 96.41%)p 0.04(  3.59%)
                                         -0.0012  0.9819 -0.0077 -0.1569  0.0352
                                          0.1001
1294. (0.00022) RY*( 2) H 103           s( 91.62%)p 0.09(  8.38%)
                                         -0.0029  0.0392  0.9564  0.0089 -0.1612
                                         -0.2402
1295. (0.00012) RY*( 3) H 103           s(  2.45%)p39.82( 97.55%)
                                         -0.0020  0.0528  0.1473  0.7316 -0.0575
                                          0.6610
1296. (0.00008) RY*( 4) H 103           s(  8.51%)p10.76( 91.49%)
1297. (0.00003) RY*( 5) H 103           s(  1.05%)p94.22( 98.95%)
1298. (0.00076) RY*( 1) H 104           s( 96.23%)p 0.04(  3.77%)
                                         -0.0023  0.9810 -0.0062 -0.1101 -0.0145
                                          0.1592
1299. (0.00022) RY*( 2) H 104           s( 69.92%)p 0.43( 30.08%)
                                         -0.0023  0.0366  0.8354 -0.1350 -0.4209
                                         -0.3247
1300. (0.00014) RY*( 3) H 104           s( 11.87%)p 7.42( 88.13%)
                                          0.0004  0.1227  0.3220  0.5663  0.6908
                                         -0.2889
1301. (0.00011) RY*( 4) H 104           s( 21.82%)p 3.58( 78.18%)
                                          0.0011 -0.1453  0.4440 -0.2232  0.3317
                                          0.7887
1302. (0.00002) RY*( 5) H 104           s(  0.21%)p99.99( 99.79%)
1303. (0.00059) RY*( 1) H 105           s( 91.25%)p 0.10(  8.75%)
                                         -0.0003  0.9552 -0.0087 -0.0226  0.1044
                                         -0.2758
1304. (0.00014) RY*( 2) H 105           s( 96.45%)p 0.04(  3.55%)
                                         -0.0029  0.0578  0.9804  0.0665 -0.1360
                                          0.1122
1305. (0.00014) RY*( 3) H 105           s(  0.15%)p99.99( 99.85%)
                                         -0.0016  0.0381 -0.0031  0.7391  0.6021
                                          0.2995
1306. (0.00006) RY*( 4) H 105           s( 10.10%)p 8.90( 89.90%)
1307. (0.00003) RY*( 5) H 105           s(  2.09%)p46.82( 97.91%)
1308. (0.00053) RY*( 1) H 106           s( 91.89%)p 0.09(  8.11%)
                                         -0.0015  0.9585 -0.0116  0.0981 -0.0296
                                         -0.2658
1309. (0.00014) RY*( 2) H 106           s( 19.04%)p 4.25( 80.96%)
                                         -0.0007  0.0488  0.4336 -0.8126  0.3416
                                         -0.1806
1310. (0.00013) RY*( 3) H 106           s( 74.09%)p 0.35( 25.91%)
                                         -0.0017  0.0704  0.8578  0.3602 -0.0539
                                          0.3556
1311. (0.00007) RY*( 4) H 106           s( 14.05%)p 6.12( 85.95%)
1312. (0.00002) RY*( 5) H 106           s(  0.99%)p99.99( 99.01%)
1313. (0.00074) RY*( 1) H 107           s( 95.58%)p 0.05(  4.42%)
                                         -0.0020  0.9775 -0.0197  0.1393  0.0514
                                         -0.1487
1314. (0.00020) RY*( 2) H 107           s( 53.99%)p 0.85( 46.01%)
                                         -0.0014  0.1013  0.7278 -0.4062  0.4268
                                          0.3361
1315. (0.00014) RY*( 3) H 107           s( 23.14%)p 3.32( 76.86%)
                                         -0.0010  0.0644  0.4767 -0.0077 -0.8752
                                          0.0504
1316. (0.00006) RY*( 4) H 107           s( 26.48%)p 2.78( 73.52%)
1317. (0.00002) RY*( 5) H 107           s(  0.85%)p99.99( 99.15%)
1318. (0.00076) RY*( 1) H 108           s( 95.72%)p 0.04(  4.28%)
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                                     -0.0007  0.9784  0.0024 -0.1621 -0.1193
                                     -0.0477
1319. (0.00018) RY*( 2) H 108       s( 44.01%)p 1.27( 55.99%)
                                     -0.0019 -0.0120  0.6633  0.0190 -0.3708
                                      0.6496
1320. (0.00013) RY*( 3) H 108       s( 51.47%)p 0.94( 48.53%)
                                     -0.0010 -0.0439  0.7161 -0.1133  0.0808
                                     -0.6826
1321. (0.00011) RY*( 4) H 108       s(  8.02%)p11.48( 91.98%)
                                     -0.0004  0.1984  0.2020  0.6359  0.6961
                                      0.1761
1322. (0.00002) RY*( 5) H 108       s(  0.82%)p99.99( 99.18%)
1323. (0.00088) RY*( 1) H 109       s( 95.98%)p 0.04(  4.02%)
                                     -0.0022  0.9797 -0.0014 -0.0197 -0.1961
                                      0.0369
1324. (0.00020) RY*( 2) H 109       s( 71.72%)p 0.39( 28.28%)
                                     -0.0023 -0.0033  0.8469 -0.4127  0.0807
                                      0.3255
1325. (0.00014) RY*( 3) H 109       s( 22.82%)p 3.38( 77.18%)
                                      0.0013  0.1024  0.4666  0.5756  0.3432
                                     -0.5681
1326. (0.00009) RY*( 4) H 109       s(  9.37%)p 9.67( 90.63%)
1327. (0.00002) RY*( 5) H 109       s(  0.16%)p99.99( 99.84%)
1328. (0.00066) RY*( 1) H 110       s( 96.01%)p 0.04(  3.99%)
                                     -0.0016  0.9798 -0.0027 -0.0626 -0.1853
                                     -0.0406
1329. (0.00024) RY*( 2) H 110       s( 85.84%)p 0.16( 14.16%)
                                     -0.0026  0.0079  0.9265 -0.3480  0.1419
                                      0.0184
1330. (0.00014) RY*( 3) H 110       s( 11.98%)p 7.34( 88.02%)
                                     -0.0010  0.0417  0.3437  0.8722 -0.1479
                                      0.3124
1331. (0.00007) RY*( 4) H 110       s(  5.10%)p18.62( 94.90%)
1332. (0.00002) RY*( 5) H 110       s(  1.11%)p89.20( 98.89%)
1333. (0.00075) RY*( 1) H 111       s( 94.88%)p 0.05(  5.12%)
                                     -0.0007  0.9741 -0.0009  0.1363  0.0626
                                     -0.1695
1334. (0.00017) RY*( 2) H 111       s(  4.59%)p20.77( 95.41%)
                                     -0.0018  0.0344  0.2116  0.0064  0.8333
                                      0.5096
1335. (0.00014) RY*( 3) H 111       s( 94.14%)p 0.06(  5.86%)
                                     -0.0025  0.0006  0.9703 -0.1120 -0.1543
                                     -0.1491
1336. (0.00009) RY*( 4) H 111       s(  4.78%)p19.92( 95.22%)
1337. (0.00002) RY*( 5) H 111       s(  1.65%)p59.54( 98.35%)
1338. (0.00085) RY*( 1) H 112       s( 96.23%)p 0.04(  3.77%)
                                     -0.0023  0.9809 -0.0086 -0.0001  0.1468
                                     -0.1272
1339. (0.00021) RY*( 2) H 112       s( 52.23%)p 0.91( 47.77%)
                                     -0.0013  0.0507  0.7209  0.5942  0.0097
                                      0.3529
1340. (0.00015) RY*( 3) H 112       s( 37.21%)p 1.69( 62.79%)
                                     -0.0004  0.0514  0.6079 -0.6556 -0.4245
                                     -0.1337
1341. (0.00008) RY*( 4) H 112       s( 14.22%)p 6.03( 85.78%)
1342. (0.00002) RY*( 5) H 112       s(  0.15%)p99.99( 99.85%)
1343. (0.00047) RY*( 1) H 113       s( 93.67%)p 0.07(  6.33%)
                                     -0.0017  0.9677 -0.0170  0.0771  0.1067
                                     -0.2144
1344. (0.00015) RY*( 2) H 113       s(  9.50%)p 9.53( 90.50%)
                                     -0.0013 -0.0191  0.3076  0.8114 -0.4925
                                     -0.0641
1345. (0.00011) RY*( 3) H 113       s( 42.66%)p 1.34( 57.34%)
                                     -0.0028  0.1975  0.6226 -0.2278 -0.0875
                                      0.7168
1346. (0.00005) RY*( 4) H 113       s( 52.91%)p 0.89( 47.09%)
1347. (0.00002) RY*( 5) H 113       s(  1.29%)p76.33( 98.71%)
1348. (0.00064) RY*( 1) H 114       s( 91.79%)p 0.09(  8.21%)
                                     -0.0004  0.9580 -0.0083 -0.0521 -0.2643
                                     -0.0976
1349. (0.00014) RY*( 2) H 114       s( 95.77%)p 0.04(  4.23%)
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                                      -0.0030  0.0607  0.9767 -0.0311  0.2024
                                      -0.0188
1350. (0.00014) RY*( 3) H 114       s(  0.20%)p99.99( 99.80%)
                                      -0.0015  0.0429  0.0117 -0.4989 -0.0655
                                       0.8630
1351. (0.00006) RY*( 4) H 114       s(  9.89%)p 9.11( 90.11%)
1352. (0.00002) RY*( 5) H 114       s(  2.39%)p40.79( 97.61%)
1353. (0.00055) RY*( 1) H 115       s( 93.07%)p 0.07(  6.93%)
                                      -0.0016  0.9646 -0.0152 -0.1695 -0.1460
                                      -0.1390
1354. (0.00013) RY*( 2) H 115       s( 81.62%)p 0.23( 18.38%)
                                      -0.0015  0.1248  0.8948  0.1645  0.2423
                                       0.3130
1355. (0.00014) RY*( 3) H 115       s(  0.64%)p99.99( 99.36%)
                                      -0.0001  0.0240  0.0766  0.7880 -0.5785
                                      -0.1948
1356. (0.00007) RY*( 4) H 115       s( 24.01%)p 3.16( 75.99%)
1357. (0.00002) RY*( 5) H 115       s(  0.70%)p99.99( 99.30%)
1358. (0.00078) RY*( 1) H 116       s( 96.09%)p 0.04(  3.91%)
                                      -0.0022  0.9802 -0.0135 -0.1598 -0.1151
                                      -0.0184
1359. (0.00018) RY*( 2) H 116       s( 65.12%)p 0.54( 34.88%)
                                      -0.0011  0.0940  0.8015  0.4968 -0.0341
                                       0.3177
1360. (0.00015) RY*( 3) H 116       s( 15.42%)p 5.49( 84.58%)
                                      -0.0007  0.0374  0.3909 -0.1784  0.6246
                                      -0.6511
1361. (0.00006) RY*( 4) H 116       s( 23.23%)p 3.30( 76.77%)
1362. (0.00002) RY*( 5) H 116       s(  0.19%)p99.99( 99.81%)
1363. (0.00063) RY*( 1) H 117       s( 92.01%)p 0.09(  7.99%)
                                      -0.0005  0.9592 -0.0097 -0.0940 -0.2634
                                       0.0413
1364. (0.00016) RY*( 2) H 117       s( 40.16%)p 1.49( 59.84%)
                                      -0.0008  0.0096  0.6336  0.7263 -0.2580
                                      -0.0658
1365. (0.00013) RY*( 3) H 117       s( 54.46%)p 0.84( 45.54%)
                                      -0.0019  0.0942  0.7319 -0.4604  0.4897
                                       0.0598
1366. (0.00006) RY*( 4) H 117       s( 12.36%)p 7.09( 87.64%)
1367. (0.00002) RY*( 5) H 117       s(  1.05%)p94.57( 98.95%)
1368. (0.00088) RY*( 1) H 118       s( 95.87%)p 0.04(  4.13%)
                                      -0.0019  0.9791 -0.0047 -0.1141 -0.0823
                                       0.1467
1369. (0.00014) RY*( 2) H 118       s(  6.40%)p14.63( 93.60%)
                                       0.0000  0.0084  0.2528  0.7356  0.1528
                                       0.6095
1370. (0.00013) RY*( 3) H 118       s( 86.45%)p 0.16( 13.55%)
                                      -0.0018  0.0593  0.9279 -0.0229  0.0321
                                      -0.3660
1371. (0.00006) RY*( 4) H 118       s( 10.84%)p 8.23( 89.16%)
1372. (0.00002) RY*( 5) H 118       s(  0.49%)p99.99( 99.51%)
1373. (0.00062) RY*( 1) H 119       s( 95.44%)p 0.05(  4.56%)
                                      -0.0021  0.9768 -0.0175 -0.0735 -0.1741
                                       0.0993
1374. (0.00015) RY*( 2) H 119       s( 49.50%)p 1.02( 50.50%)
                                      -0.0038  0.1316  0.6911 -0.0904  0.7049
                                      -0.0040
1375. (0.00015) RY*( 3) H 119       s( 15.28%)p 5.54( 84.72%)
                                      -0.0008  0.0287  0.3899  0.0703 -0.3833
                                      -0.8338
1376. (0.00005) RY*( 4) H 119       s( 38.94%)p 1.57( 61.06%)
1377. (0.00002) RY*( 5) H 119       s(  0.88%)p99.99( 99.12%)
1378. (0.00056) RY*( 1) H 120       s( 92.85%)p 0.08(  7.15%)
                                      -0.0007  0.9636 -0.0026  0.2373 -0.1194
                                       0.0308
1379. (0.00017) RY*( 2) H 120       s( 40.40%)p 1.47( 59.60%)
                                      -0.0026  0.0395  0.6344  0.2283  0.7266
                                      -0.1261
1380. (0.00013) RY*( 3) H 120       s( 59.66%)p 0.68( 40.34%)
                                       0.0010 -0.0202  0.7721 -0.2192 -0.5813
                                       0.1319
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1381. (0.00008) RY*( 4) H 120           s(  6.94%)p13.41( 93.06%)
1382. (0.00002) RY*( 5) H 120           s(  0.19%)p99.99( 99.81%)
1383. (0.00083) RY*( 1) H 121           s( 95.04%)p 0.05(  4.96%)
                                         -0.0012  0.9749 -0.0023  0.2019 -0.0925
                                          0.0172
1384. (0.00020) RY*( 2) H 121           s( 94.64%)p 0.06(  5.36%)
                                         -0.0030  0.0234  0.9725 -0.0096  0.2165
                                          0.0818
1385. (0.00013) RY*( 3) H 121           s(  4.71%)p20.25( 95.29%)
                                          0.0014 -0.0767  0.2029  0.1534 -0.6164
                                         -0.7413
1386. (0.00006) RY*( 4) H 121           s(  4.38%)p21.85( 95.62%)
1387. (0.00002) RY*( 5) H 121           s(  1.28%)p77.08( 98.72%)
1388. (0.00073) RY*( 1) H 122           s( 96.06%)p 0.04(  3.94%)
                                         -0.0015  0.9800 -0.0140  0.1533  0.0794
                                          0.0978
1389. (0.00025) RY*( 2) H 122           s( 67.30%)p 0.49( 32.70%)
                                         -0.0030  0.0548  0.8185  0.0880 -0.0060
                                         -0.5650
1390. (0.00013) RY*( 3) H 122           s( 12.82%)p 6.80( 87.18%)
                                         -0.0006  0.1157  0.3389 -0.7603 -0.3786
                                          0.3878
1391. (0.00009) RY*( 4) H 122           s( 20.72%)p 3.83( 79.28%)
1392. (0.00002) RY*( 5) H 122           s(  3.14%)p30.87( 96.86%)
1393. (0.00070) RY*( 1) H 123           s( 94.88%)p 0.05(  5.12%)
                                         -0.0007  0.9740 -0.0061  0.0542  0.1679
                                          0.1418
1394. (0.00020) RY*( 2) H 123           s( 28.86%)p 2.46( 71.14%)
                                         -0.0014  0.0564  0.5343  0.5548  0.0481
                                         -0.6334
1395. (0.00012) RY*( 3) H 123           s( 69.75%)p 0.43( 30.25%)
                                         -0.0007  0.0037  0.8351 -0.3809 -0.1710
                                          0.3581
1396. (0.00007) RY*( 4) H 123           s(  6.38%)p14.66( 93.62%)
1397. (0.00003) RY*( 5) H 123           s(  0.17%)p99.99( 99.83%)
1398. (0.00073) RY*( 1) H 124           s( 95.65%)p 0.05(  4.35%)
                                         -0.0017  0.9778 -0.0183  0.1844  0.0750
                                          0.0625
1399. (0.00024) RY*( 2) H 124           s( 62.30%)p 0.61( 37.70%)
                                         -0.0022  0.0808  0.7852 -0.3389  0.3100
                                         -0.4075
1400. (0.00012) RY*( 3) H 124           s( 19.04%)p 4.25( 80.96%)
                                         -0.0011  0.0767  0.4295 -0.2182 -0.7419
                                          0.4600
1401. (0.00008) RY*( 4) H 124           s( 18.24%)p 4.48( 81.76%)
1402. (0.00002) RY*( 5) H 124           s(  4.81%)p19.79( 95.19%)
1403. (0.00056) RY*( 1) H 125           s( 93.15%)p 0.07(  6.85%)
                                         -0.0015  0.9652 -0.0026  0.0731  0.1790
                                          0.1763
1404. (0.00017) RY*( 2) H 125           s( 30.00%)p 2.33( 70.00%)
                                         -0.0015  0.0684  0.5434  0.6225 -0.5557
                                         -0.0601
1405. (0.00014) RY*( 3) H 125           s( 69.77%)p 0.43( 30.23%)
                                         -0.0014 -0.0342  0.8346 -0.3715  0.4017
                                         -0.0543
1406. (0.00007) RY*( 4) H 125           s(  6.31%)p14.84( 93.69%)
1407. (0.00002) RY*( 5) H 125           s(  0.80%)p99.99( 99.20%)
1408. (0.00062) RY*( 1) H 126           s( 91.71%)p 0.09(  8.29%)
                                         -0.0004  0.9576 -0.0104 -0.2351 -0.0549
                                          0.1568
1409. (0.00016) RY*( 2) H 126           s( 39.90%)p 1.51( 60.10%)
                                         -0.0007  0.0148  0.6315  0.1376  0.6568
                                          0.3882
1410. (0.00012) RY*( 3) H 126           s( 54.50%)p 0.83( 45.50%)
                                         -0.0019  0.0945  0.7322  0.1691 -0.4797
                                         -0.4430
1411. (0.00006) RY*( 4) H 126           s( 12.96%)p 6.71( 87.04%)
1412. (0.00002) RY*( 5) H 126           s(  0.96%)p99.99( 99.04%)
1413. (0.00062) RY*( 1) H 127           s( 95.91%)p 0.04(  4.09%)
                                         -0.0024  0.9791 -0.0197 -0.1305 -0.0877
                                          0.1271
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1414. (0.00017) RY*( 2) H 127           s( 58.58%)p 0.71( 41.42%)
                                         -0.0045  0.1288  0.7545  0.2689  0.0212
                                         -0.5843
1415. (0.00015) RY*( 3) H 127           s(  3.22%)p30.07( 96.78%)
                                          0.0006 -0.0267  0.1774 -0.7474  0.6321
                                         -0.0979
1416. (0.00005) RY*( 4) H 127           s( 41.14%)p 1.43( 58.86%)
1417. (0.00002) RY*( 5) H 127           s(  1.19%)p82.93( 98.81%)
1418. (0.00088) RY*( 1) H 128           s( 95.49%)p 0.05(  4.51%)
                                         -0.0019  0.9772 -0.0055 -0.0592 -0.1700
                                          0.1126
1419. (0.00015) RY*( 2) H 128           s(  5.84%)p16.14( 94.16%)
                                         -0.0001  0.0062  0.2415  0.7301  0.1803
                                          0.6133
1420. (0.00013) RY*( 3) H 128           s( 86.00%)p 0.16( 14.00%)
                                         -0.0020  0.0671  0.9249 -0.1283  0.2176
                                         -0.2761
1421. (0.00006) RY*( 4) H 128           s( 12.01%)p 7.32( 87.99%)
1422. (0.00002) RY*( 5) H 128           s(  0.71%)p99.99( 99.29%)
1423. (0.00064) RY*( 1) H 129           s( 91.66%)p 0.09(  8.34%)
                                         -0.0004  0.9573 -0.0088 -0.2729  0.0629
                                          0.0710
1424. (0.00014) RY*( 2) H 129           s( 95.22%)p 0.05(  4.78%)
                                         -0.0025  0.0636  0.9737  0.1535  0.0099
                                         -0.1553
1425. (0.00015) RY*( 3) H 129           s(  0.59%)p99.99( 99.41%)
                                         -0.0014  0.0466  0.0609  0.0543 -0.9132
                                          0.3965
1426. (0.00006) RY*( 4) H 129           s( 10.82%)p 8.24( 89.18%)
1427. (0.00002) RY*( 5) H 129           s(  1.76%)p55.94( 98.24%)
1428. (0.00079) RY*( 1) H 130           s( 96.11%)p 0.04(  3.89%)
                                         -0.0022  0.9803 -0.0121 -0.1737 -0.0915
                                         -0.0182
1429. (0.00017) RY*( 2) H 130           s( 73.07%)p 0.37( 26.93%)
                                         -0.0014  0.0925  0.8498  0.3259  0.1899
                                          0.3564
1430. (0.00015) RY*( 3) H 130           s( 10.00%)p 9.00( 90.00%)
                                         -0.0006  0.0186  0.3156  0.0981  0.1567
                                         -0.9305
1431. (0.00006) RY*( 4) H 130           s( 20.56%)p 3.86( 79.44%)
1432. (0.00002) RY*( 5) H 130           s(  0.31%)p99.99( 99.69%)
1433. (0.00059) RY*( 1) H 131           s( 95.06%)p 0.05(  4.94%)
                                         -0.0017  0.9749 -0.0136 -0.2171 -0.0082
                                         -0.0466
1434. (0.00013) RY*( 2) H 131           s( 72.41%)p 0.38( 27.59%)
                                         -0.0016  0.1270  0.8414  0.4642  0.0152
                                          0.2454
1435. (0.00014) RY*( 3) H 131           s(  0.46%)p99.99( 99.54%)
                                         -0.0004  0.0105  0.0669  0.1911 -0.8129
                                         -0.5460
1436. (0.00007) RY*( 4) H 131           s( 31.52%)p 2.17( 68.48%)
1437. (0.00002) RY*( 5) H 131           s(  0.59%)p99.99( 99.41%)
1438. (0.00076) RY*( 1) H 132           s( 95.71%)p 0.04(  4.29%)
                                         -0.0006  0.9783  0.0039  0.0088  0.1903
                                         -0.0812
1439. (0.00018) RY*( 2) H 132           s( 52.73%)p 0.90( 47.27%)
                                         -0.0022 -0.0148  0.7260  0.6235 -0.0856
                                         -0.2767
1440. (0.00014) RY*( 3) H 132           s( 43.30%)p 1.31( 56.70%)
                                         -0.0001 -0.0442  0.6565 -0.6977  0.2750
                                          0.0677
1441. (0.00009) RY*( 4) H 132           s(  7.55%)p12.25( 92.45%)
1442. (0.00002) RY*( 5) H 132           s(  0.75%)p99.99( 99.25%)
1443. (0.00092) RY*( 1) H 133           s( 96.52%)p 0.04(  3.48%)
                                         -0.0019  0.9824 -0.0002  0.0221  0.1030
                                         -0.1540
1444. (0.00023) RY*( 2) H 133           s( 93.67%)p 0.07(  6.33%)
                                         -0.0015  0.0041  0.9678  0.0292  0.1933
                                          0.1584
1445. (0.00013) RY*( 3) H 133           s(  5.98%)p15.71( 94.02%)
                                          0.0005  0.0113  0.2444  0.0648 -0.8396
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                                        -0.4807
1446. (0.00008) RY*( 4) H 133           s(  3.56%)p27.13( 96.44%)
1447. (0.00002) RY*( 5) H 133           s(  0.31%)p99.99( 99.69%)
1448. (0.00075) RY*( 1) H 134           s( 96.00%)p 0.04(  4.00%)
                                         -0.0023  0.9797 -0.0103  0.0551  0.0567
                                         -0.1838
1449. (0.00021) RY*( 2) H 134           s( 69.49%)p 0.44( 30.51%)
                                         -0.0021  0.0575  0.8316  0.2961  0.2132
                                          0.4147
1450. (0.00014) RY*( 3) H 134           s( 14.94%)p 5.69( 85.06%)
                                          0.0003  0.0829  0.3776 -0.7947 -0.4665
                                          0.0387
1451. (0.00009) RY*( 4) H 134           s( 19.45%)p 4.14( 80.55%)
1452. (0.00002) RY*( 5) H 134           s(  0.17%)p99.99( 99.83%)
1453. (0.04220) BD*( 1) C   1 - O   2
              ( 64.58%)   0.8036* C   1 s( 34.37%)p 1.91( 65.56%)d 0.00(  0.06%)
                                         -0.0003  0.5810  0.0787  0.0026  0.0008
                                         -0.1509  0.0180 -0.0037  0.2199 -0.0122
                                          0.0042 -0.7618  0.0561 -0.0225 -0.0018
                                          0.0052 -0.0118 -0.0016  0.0209
              ( 35.42%)  -0.5952* O   2 s( 39.92%)p 1.50( 59.94%)d 0.00(  0.14%)
                                          0.0000  0.6315 -0.0188  0.0010  0.0004
                                          0.1663 -0.0065  0.0004 -0.1629  0.0093
                                         -0.0006  0.7377 -0.0308  0.0019 -0.0037
                                          0.0129 -0.0137 -0.0010  0.0316
1454. (0.48062) BD*( 2) C   1 - O   2
              ( 73.22%)   0.8557* C   1 s(  0.01%)p99.99( 99.72%)d18.73(  0.27%)
                                          0.0002 -0.0112 -0.0035 -0.0020 -0.0003
                                         -0.2669  0.0057  0.0009  0.9119 -0.0046
                                          0.0006  0.3072 -0.0019  0.0018 -0.0103
                                          0.0104 -0.0412 -0.0105 -0.0253
              ( 26.78%)  -0.5175* O   2 s(  0.02%)p99.99( 99.88%)d 5.56(  0.10%)
                                          0.0000 -0.0134 -0.0014 -0.0001  0.0000
                                         -0.2373  0.0040  0.0009  0.9322 -0.0117
                                         -0.0030  0.2709 -0.0019 -0.0007  0.0081
                                         -0.0058  0.0259  0.0058  0.0143
1455. (0.11075) BD*( 1) C   1 - B  14
              ( 39.95%)   0.6321* C   1 s( 25.83%)p 2.87( 74.14%)d 0.00(  0.03%)
                                          0.0001 -0.5076  0.0246  0.0070  0.0004
                                         -0.8031 -0.0080  0.0050 -0.1500  0.0005
                                         -0.0048 -0.2708 -0.0196  0.0097 -0.0031
                                         -0.0135  0.0001 -0.0090 -0.0021
              ( 60.05%)  -0.7749* B  14 s( 18.02%)p 4.55( 81.92%)d 0.00(  0.06%)
                                          0.0048 -0.4244 -0.0071  0.0015  0.0003
                                          0.4109 -0.0053  0.0033 -0.0158 -0.0057
                                         -0.0025  0.8062  0.0060  0.0081 -0.0063
                                         -0.0176  0.0066 -0.0089 -0.0131
1456. (0.06815) BD*( 1) C   1 - B  15
              ( 39.01%)   0.6246* C   1 s( 40.15%)p 1.49( 59.83%)d 0.00(  0.02%)
                                         -0.0001  0.6328 -0.0332  0.0034 -0.0001
                                         -0.5101 -0.0005 -0.0070 -0.3077 -0.0062
                                         -0.0019  0.4931  0.0133 -0.0081  0.0030
                                         -0.0054 -0.0082 -0.0022  0.0088
              ( 60.99%)  -0.7810* B  15 s( 26.26%)p 2.81( 73.68%)d 0.00(  0.06%)
                                         -0.0013  0.5124 -0.0006  0.0061  0.0024
                                         -0.1733 -0.0148 -0.0020  0.2436 -0.0080
                                          0.0044 -0.8041  0.0048 -0.0218  0.0056
                                          0.0010 -0.0151 -0.0019  0.0182
1457. (0.03587) BD*( 1) C   3 - C   4
              ( 50.75%)   0.7124* C   3 s( 33.55%)p 1.98( 66.40%)d 0.00(  0.05%)
                                          0.0000  0.5792  0.0032 -0.0011  0.0000
                                          0.6350  0.0004  0.0019 -0.3736  0.0069
                                         -0.0003  0.3477  0.0118 -0.0009 -0.0140
                                          0.0145 -0.0072  0.0091 -0.0030
              ( 49.25%)  -0.7018* C   4 s( 36.74%)p 1.72( 63.22%)d 0.00(  0.05%)
                                         -0.0002  0.6061 -0.0011 -0.0031  0.0001
                                         -0.6195 -0.0040  0.0023  0.3295  0.0077
                                          0.0040 -0.3739  0.0032  0.0010 -0.0129
                                          0.0138 -0.0072  0.0075 -0.0019
1458. (0.02327) BD*( 1) C   3 - C   8
              ( 49.58%)   0.7041* C   3 s( 34.07%)p 1.93( 65.88%)d 0.00(  0.05%)
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                                        0.0001 -0.5836 -0.0091 -0.0048 -0.0002
                                        0.4788 -0.0077  0.0076 -0.4929  0.0029
                                       -0.0080 -0.4318 -0.0076  0.0010  0.0138
                                        0.0104 -0.0129  0.0009 -0.0007
              ( 50.42%)  -0.7101* C   8 s( 35.90%)p 1.78( 64.04%)d 0.00(  0.06%)
                                       -0.0001 -0.5992  0.0007  0.0043  0.0002
                                       -0.4507  0.0025  0.0059  0.4802  0.0069
                                       -0.0071  0.4539  0.0196 -0.0025  0.0166
                                        0.0120 -0.0142 -0.0003  0.0001
1459. (0.33135) BD*( 2) C   3 - C   8
              ( 52.21%)   0.7226* C   3 s(  0.01%)p 1.00( 99.96%)d 0.00(  0.04%)
                                       -0.0002 -0.0061 -0.0052  0.0017  0.0003
                                        0.5871 -0.0051 -0.0041  0.7766 -0.0049
                                        0.0038 -0.2274  0.0013  0.0034  0.0020
                                        0.0102  0.0115 -0.0080 -0.0077
              ( 47.79%)  -0.6913* C   8 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                        0.0000 -0.0005  0.0012 -0.0001  0.0005
                                        0.5811 -0.0025  0.0077  0.7759 -0.0046
                                        0.0117 -0.2444  0.0029 -0.0050  0.0039
                                       -0.0044  0.0011  0.0165  0.0008
1460. (0.03220) BD*( 1) C   3 - C  53
              ( 49.42%)   0.7030* C   3 s( 32.34%)p 2.09( 67.63%)d 0.00(  0.03%)
                                        0.0001 -0.5687  0.0066  0.0047  0.0002
                                        0.1492  0.0019  0.0020  0.1170 -0.0003
                                       -0.0019  0.8000  0.0171 -0.0075  0.0010
                                       -0.0041 -0.0037 -0.0004 -0.0167
              ( 50.58%)  -0.7112* C  53 s( 26.35%)p 2.79( 73.59%)d 0.00(  0.06%)
                                       -0.0002 -0.5134  0.0001 -0.0003 -0.0007
                                       -0.1312  0.0019  0.0018 -0.1039  0.0049
                                       -0.0005 -0.8413  0.0005 -0.0012 -0.0017
                                       -0.0071 -0.0055 -0.0001 -0.0222
1461. (0.03690) BD*( 1) C   4 - C   5
              ( 49.60%)   0.7043* C   4 s( 36.67%)p 1.73( 63.29%)d 0.00(  0.05%)
                                        0.0002 -0.6055  0.0021  0.0024 -0.0002
                                       -0.1961  0.0018  0.0000 -0.1188 -0.0073
                                       -0.0029 -0.7617 -0.0054 -0.0009 -0.0001
                                       -0.0098 -0.0064 -0.0016 -0.0184
              ( 50.40%)  -0.7100* C   5 s( 34.19%)p 1.92( 65.76%)d 0.00(  0.05%)
                                        0.0000 -0.5847 -0.0024  0.0005  0.0000
                                        0.1664  0.0103 -0.0024  0.1615 -0.0086
                                        0.0002  0.7770  0.0013  0.0000  0.0001
                                       -0.0093 -0.0063 -0.0014 -0.0199
1462. (0.37359) BD*( 2) C   4 - C   5
              ( 46.53%)   0.6821* C   4 s(  0.01%)p 1.00( 99.97%)d 0.00(  0.02%)
                                        0.0002  0.0074  0.0051 -0.0012 -0.0002
                                       -0.5662  0.0040  0.0069 -0.7814  0.0019
                                        0.0052  0.2617 -0.0052 -0.0035 -0.0036
                                       -0.0068 -0.0089  0.0036  0.0072
              ( 53.47%)  -0.7313* C   5 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                        0.0000  0.0033  0.0047 -0.0017 -0.0001
                                       -0.5493  0.0052  0.0024 -0.7857  0.0081
                                        0.0027  0.2835 -0.0007  0.0017  0.0075
                                        0.0073  0.0147  0.0077 -0.0082
1463. (0.03921) BD*( 1) C   4 - N   9
              ( 62.34%)   0.7896* C   4 s( 26.55%)p 2.76( 73.39%)d 0.00(  0.06%)
                                       -0.0002  0.5151  0.0074  0.0066 -0.0005
                                        0.5066  0.0050  0.0081 -0.5159 -0.0055
                                       -0.0090 -0.4593  0.0016 -0.0076 -0.0161
                                       -0.0134  0.0140  0.0008 -0.0009
              ( 37.66%)  -0.6136* N   9 s( 34.35%)p 1.91( 65.61%)d 0.00(  0.04%)
                                       -0.0001  0.5861  0.0014 -0.0018 -0.0002
                                       -0.5033 -0.0022  0.0070  0.4858  0.0043
                                       -0.0067  0.4082 -0.0003 -0.0048 -0.0105
                                       -0.0123  0.0112 -0.0002 -0.0016
1464. (0.02290) BD*( 1) C   5 - C   6
              ( 49.51%)   0.7036* C   5 s( 33.92%)p 1.95( 66.03%)d 0.00(  0.05%)
                                        0.0001 -0.5823 -0.0106 -0.0031 -0.0001
                                        0.4752  0.0025  0.0010 -0.4927  0.0003
                                       -0.0048 -0.4376  0.0094 -0.0090  0.0150
                                        0.0100 -0.0120 -0.0004  0.0013
              ( 50.49%)  -0.7106* C   6 s( 35.81%)p 1.79( 64.13%)d 0.00(  0.06%)
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                                     -0.0001 -0.5984  0.0016  0.0044  0.0001
                                     -0.4925 -0.0164  0.0051  0.4866  0.0112
                                     -0.0066  0.4018 -0.0051 -0.0076  0.0168
                                      0.0117 -0.0137 -0.0007  0.0004
1465. (0.03210) BD*( 1) C   5 - C  51
              ( 49.98%)   0.7070* C   5 s( 31.86%)p 2.14( 68.11%)d 0.00(  0.03%)
                                      0.0001 -0.5644  0.0069  0.0033  0.0000
                                     -0.6662 -0.0130  0.0046  0.3364  0.0053
                                     -0.0026 -0.3517 -0.0096  0.0018  0.0105
                                     -0.0103  0.0041 -0.0084  0.0036
              ( 50.02%)  -0.7072* C  51 s( 26.67%)p 2.75( 73.28%)d 0.00(  0.06%)
                                     -0.0001 -0.5164 -0.0015  0.0019  0.0002
                                      0.7022 -0.0010 -0.0024 -0.3264  0.0035
                                      0.0000  0.3649  0.0009 -0.0026  0.0128
                                     -0.0144  0.0069 -0.0104  0.0054
1466. (0.01486) BD*( 1) C   6 - C   7
              ( 49.78%)   0.7056* C   6 s( 36.09%)p 1.77( 63.85%)d 0.00(  0.05%)
                                      0.0000 -0.6006 -0.0147 -0.0044 -0.0001
                                      0.6446  0.0175  0.0032 -0.3477 -0.0183
                                     -0.0066  0.3178 -0.0155 -0.0120  0.0115
                                     -0.0161  0.0067 -0.0089  0.0006
              ( 50.22%)  -0.7086* C   7 s( 35.95%)p 1.78( 63.98%)d 0.00(  0.07%)
                                      0.0000 -0.5996 -0.0077  0.0016  0.0001
                                     -0.6232 -0.0103  0.0093  0.3357 -0.0025
                                     -0.0091 -0.3708 -0.0309 -0.0057  0.0182
                                     -0.0120  0.0058 -0.0096  0.0073
1467. (0.33555) BD*( 2) C   6 - C   7
              ( 48.96%)   0.6997* C   6 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                                      0.0000 -0.0015  0.0002 -0.0006 -0.0001
                                     -0.5570  0.0058 -0.0136 -0.7859  0.0076
                                     -0.0176  0.2669 -0.0028  0.0054  0.0053
                                      0.0049  0.0103  0.0058 -0.0060
              ( 51.04%)  -0.7144* C   7 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                      0.0000 -0.0039  0.0000 -0.0013 -0.0001
                                     -0.5698  0.0063 -0.0060 -0.7800  0.0074
                                     -0.0096  0.2578 -0.0028  0.0028 -0.0044
                                      0.0034 -0.0027 -0.0148 -0.0002
1468. (0.01759) BD*( 1) C   6 - H  78
              ( 39.24%)   0.6264* C   6 s( 28.07%)p 2.56( 71.90%)d 0.00(  0.04%)
                                      0.0004 -0.5297  0.0109  0.0003 -0.0001
                                     -0.1735  0.0082  0.0044 -0.1530 -0.0002
                                      0.0007 -0.8155  0.0142  0.0126 -0.0010
                                     -0.0071 -0.0057 -0.0003 -0.0168
              ( 60.76%)  -0.7795* H  78 s( 99.95%)p 0.00(  0.05%)
                                     -0.9997 -0.0022 -0.0013  0.0050  0.0040
                                      0.0222
1469. (0.01498) BD*( 1) C   7 - C   8
              ( 50.04%)   0.7074* C   7 s( 36.04%)p 1.77( 63.89%)d 0.00(  0.06%)
                                      0.0000  0.6003  0.0063 -0.0024 -0.0002
                                     -0.1853 -0.0243 -0.0055 -0.1213  0.0118
                                      0.0094 -0.7672 -0.0174  0.0095 -0.0005
                                      0.0050  0.0105 -0.0005  0.0226
              ( 49.96%)  -0.7069* C   8 s( 35.83%)p 1.79( 64.12%)d 0.00(  0.05%)
                                      0.0000  0.5984  0.0139  0.0046  0.0002
                                      0.1372 -0.0176 -0.0093  0.1417  0.0186
                                      0.0098  0.7754  0.0163  0.0012 -0.0001
                                      0.0115  0.0031  0.0019  0.0191
1470. (0.01576) BD*( 1) C   7 - H  77
              ( 39.16%)   0.6258* C   7 s( 27.95%)p 2.58( 72.01%)d 0.00(  0.03%)
                                     -0.0004  0.5286 -0.0118  0.0036  0.0003
                                     -0.5010  0.0133 -0.0018  0.5131 -0.0144
                                      0.0026  0.4530 -0.0128  0.0024 -0.0076
                                     -0.0127  0.0092 -0.0020 -0.0041
              ( 60.84%)  -0.7800* H  77 s( 99.95%)p 0.00(  0.05%)
                                      0.9997  0.0015  0.0005  0.0136 -0.0141
                                     -0.0123
1471. (0.01781) BD*( 1) C   8 - H  76
              ( 38.92%)   0.6238* C   8 s( 28.24%)p 2.54( 71.73%)d 0.00(  0.04%)
                                     -0.0004  0.5313 -0.0108 -0.0006  0.0001
                                     -0.6628  0.0102  0.0096  0.3826 -0.0062
                                     -0.0030 -0.3622  0.0106  0.0065 -0.0115
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                                      0.0112 -0.0063  0.0070 -0.0039
              ( 61.08%)  -0.7816* H  76 s( 99.95%)p 0.00(  0.05%)
                                      0.9997 -0.0020  0.0015  0.0184 -0.0096
                                      0.0106
1472. (0.04581) BD*( 1) N   9 - C  10
              ( 37.53%)   0.6126* N   9 s( 33.77%)p 1.96( 66.17%)d 0.00(  0.05%)
                                     -0.0001  0.5812 -0.0006  0.0005  0.0001
                                     -0.1567  0.0128 -0.0030 -0.7937  0.0065
                                      0.0042 -0.0829 -0.0075  0.0023  0.0033
                                     -0.0015  0.0045 -0.0191 -0.0116
              ( 62.47%)  -0.7904* C  10 s( 26.30%)p 2.80( 73.64%)d 0.00(  0.06%)
                                     -0.0004  0.5123  0.0205  0.0092 -0.0005
                                      0.0496 -0.0115 -0.0041  0.8485  0.0207
                                      0.0158  0.1141  0.0057  0.0065  0.0078
                                     -0.0005  0.0007 -0.0195 -0.0135
1473. (0.72110) BD*( 2) N   9 - C  10
              ( 23.81%)   0.4879* N   9 s(  0.08%)p99.99( 99.90%)d 0.16(  0.01%)
                                      0.0001  0.0286 -0.0055  0.0002  0.0000
                                     -0.4677 -0.0066 -0.0033  0.2030  0.0001
                                      0.0017 -0.8596 -0.0076 -0.0085  0.0057
                                     -0.0023  0.0086 -0.0003  0.0047
              ( 76.19%)  -0.8729* C  10 s(  0.09%)p99.99( 99.74%)d 1.76(  0.17%)
                                     -0.0003 -0.0299 -0.0060  0.0037 -0.0003
                                     -0.4290  0.0003 -0.0060  0.1623  0.0095
                                     -0.0087 -0.8865 -0.0299  0.0064 -0.0161
                                     -0.0117 -0.0336 -0.0113 -0.0020
1474. (0.03014) BD*( 1) N   9 - C  13
              ( 38.02%)   0.6166* N   9 s( 31.75%)p 2.15( 68.20%)d 0.00(  0.05%)
                                      0.0001 -0.5634  0.0047 -0.0013 -0.0001
                                     -0.7088  0.0056  0.0011 -0.3030  0.0236
                                     -0.0050  0.2953 -0.0059  0.0005 -0.0098
                                      0.0129  0.0026 -0.0134  0.0081
              ( 61.98%)  -0.7873* C  13 s( 28.26%)p 2.54( 71.68%)d 0.00(  0.05%)
                                      0.0001 -0.5316 -0.0032 -0.0003  0.0016
                                      0.7547  0.0287  0.0054  0.1846 -0.0096
                                     -0.0080 -0.3346 -0.0139  0.0005 -0.0120
                                      0.0141  0.0041 -0.0101  0.0092
1475. (0.04659) BD*( 1) C  10 - N  11
              ( 62.47%)   0.7904* C  10 s( 26.68%)p 2.75( 73.25%)d 0.00(  0.07%)
                                      0.0003 -0.5161 -0.0213 -0.0043 -0.0005
                                     -0.6918 -0.0103 -0.0069  0.2967  0.0190
                                      0.0109  0.4064  0.0119  0.0035  0.0066
                                      0.0197 -0.0043 -0.0148  0.0043
              ( 37.53%)  -0.6126* N  11 s( 34.03%)p 1.94( 65.91%)d 0.00(  0.05%)
                                      0.0001 -0.5834  0.0016  0.0010 -0.0001
                                      0.7080 -0.0084 -0.0014 -0.1705 -0.0128
                                      0.0062 -0.3585  0.0042  0.0015  0.0095
                                      0.0166 -0.0055 -0.0109  0.0048
1476. (0.02957) BD*( 1) C  10 - B  14
              ( 33.22%)   0.5763* C  10 s( 46.95%)p 1.13( 53.05%)d 0.00(  0.01%)
                                     -0.0001  0.6850 -0.0155 -0.0068 -0.0001
                                     -0.5768  0.0305  0.0040 -0.4040  0.0161
                                      0.0044  0.1823 -0.0052 -0.0044  0.0050
                                     -0.0025  0.0008  0.0025 -0.0069
              ( 66.78%)  -0.8172* B  14 s( 40.37%)p 1.48( 59.58%)d 0.00(  0.05%)
                                     -0.0004  0.6352 -0.0007  0.0122  0.0023
                                      0.6817  0.0097  0.0209  0.3609  0.0041
                                      0.0118 -0.0061  0.0050  0.0015  0.0169
                                     -0.0041 -0.0030  0.0093 -0.0109
1477. (0.02954) BD*( 1) N  11 - C  12
              ( 38.03%)   0.6167* N  11 s( 31.51%)p 2.17( 68.44%)d 0.00(  0.05%)
                                      0.0001 -0.5613  0.0035  0.0002 -0.0001
                                     -0.5370  0.0192 -0.0027 -0.6123  0.0020
                                      0.0030  0.1432 -0.0151  0.0031 -0.0183
                                      0.0038  0.0031  0.0049  0.0122
              ( 61.97%)  -0.7872* C  12 s( 28.22%)p 2.54( 71.71%)d 0.00(  0.06%)
                                      0.0001 -0.5312 -0.0034 -0.0015  0.0012
                                      0.4570  0.0049 -0.0039  0.7044  0.0333
                                      0.0062 -0.1045  0.0039  0.0063 -0.0193
                                      0.0078  0.0050  0.0033  0.0130
1478. (0.03975) BD*( 1) N  11 - C  41
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              ( 37.63%)   0.6135* N  11 s( 34.36%)p 1.91( 65.60%)d 0.00(  0.04%)
                                        0.0001 -0.5862 -0.0010 -0.0012  0.0002
                                       -0.2057 -0.0034  0.0033  0.7610  0.0028
                                       -0.0091  0.1858  0.0035 -0.0033  0.0086
                                        0.0031 -0.0054  0.0132  0.0101
              ( 62.37%)  -0.7897* C  41 s( 26.52%)p 2.77( 73.36%)d 0.00(  0.12%)
                                        0.0002 -0.5149 -0.0047 -0.0051  0.0006
                                        0.2723  0.0053 -0.0002 -0.7932  0.0014
                                       -0.0077 -0.1726  0.0195 -0.0063  0.0216
                                       -0.0013  0.0086  0.0195  0.0170
1479. (0.45441) BD*( 2) N  11 - C  41
              (  1.54%)   0.1241* N  11 s(  0.05%)p99.99( 99.95%)d 0.07(  0.00%)
                                        0.0002  0.0219 -0.0041  0.0000  0.0000
                                       -0.4088 -0.0051 -0.0039  0.1270 -0.0003
                                        0.0017 -0.9034 -0.0040 -0.0089 -0.0025
                                       -0.0014 -0.0047  0.0000 -0.0026
              ( 98.46%)  -0.9923* C  41 s(  1.14%)p58.44( 66.45%)d28.50( 32.41%)
                                       -0.0006 -0.0261 -0.0961 -0.0380 -0.0044
                                       -0.2042 -0.1381  0.0950  0.0584  0.0396
                                       -0.0642 -0.6365 -0.4107  0.1088 -0.2537
                                        0.0832 -0.4746 -0.0335 -0.1627
1480. (0.00980) BD*( 1) C  12 - C  13
              ( 50.01%)   0.7072* C  12 s( 37.54%)p 1.66( 62.40%)d 0.00(  0.05%)
                                        0.0000  0.6126  0.0104  0.0031  0.0006
                                       -0.2903  0.0129  0.0145  0.6870  0.0316
                                        0.0095  0.2575 -0.0015 -0.0065 -0.0138
                                       -0.0098  0.0116 -0.0063 -0.0088
              ( 49.99%)  -0.7070* C  13 s( 37.53%)p 1.66( 62.42%)d 0.00(  0.05%)
                                        0.0000  0.6125  0.0100  0.0033  0.0007
                                        0.4344  0.0312  0.0123 -0.5810  0.0004
                                        0.0120 -0.3106 -0.0146 -0.0068 -0.0117
                                       -0.0077  0.0113 -0.0105 -0.0100
1481. (0.28111) BD*( 2) C  12 - C  13
              ( 50.00%)   0.7071* C  12 s(  0.00%)p 1.00( 99.94%)d 0.00(  0.06%)
                                        0.0000 -0.0008 -0.0050  0.0014  0.0001
                                        0.4327 -0.0088 -0.0005 -0.1495  0.0032
                                        0.0009  0.8884 -0.0214  0.0006  0.0094
                                       -0.0085  0.0127 -0.0041  0.0156
              ( 50.00%)  -0.7071* C  13 s(  0.00%)p 1.00( 99.94%)d 0.00(  0.06%)
                                        0.0000  0.0009 -0.0060  0.0030  0.0001
                                        0.4317 -0.0092  0.0002 -0.1515  0.0050
                                       -0.0009  0.8886 -0.0207 -0.0004 -0.0107
                                        0.0030 -0.0186  0.0000 -0.0108
1482. (0.01213) BD*( 1) C  12 - H  71
              ( 38.05%)   0.6168* C  12 s( 34.17%)p 1.93( 65.81%)d 0.00(  0.02%)
                                        0.0003 -0.5845  0.0079  0.0037 -0.0002
                                       -0.7203  0.0114 -0.0016  0.0807 -0.0051
                                       -0.0116  0.3639 -0.0070 -0.0004  0.0028
                                        0.0105 -0.0017 -0.0096  0.0034
              ( 61.95%)  -0.7871* H  71 s( 99.93%)p 0.00(  0.07%)
                                       -0.9997 -0.0018 -0.0002  0.0228 -0.0029
                                       -0.0117
1483. (0.01229) BD*( 1) C  13 - H  72
              ( 38.06%)   0.6169* C  13 s( 34.15%)p 1.93( 65.83%)d 0.00(  0.02%)
                                        0.0003 -0.5843  0.0076  0.0032 -0.0005
                                       -0.2301  0.0005 -0.0092 -0.7776  0.0141
                                        0.0024 -0.0202  0.0012  0.0069 -0.0068
                                        0.0005 -0.0012  0.0107  0.0079
              ( 61.94%)  -0.7870* H  72 s( 99.93%)p 0.00(  0.07%)
                                       -0.9997 -0.0018 -0.0003  0.0071  0.0249
                                        0.0005
1484. (0.04014) BD*( 1) B  14 - B  15
              ( 50.00%)   0.7071* B  14 s( 41.46%)p 1.41( 58.51%)d 0.00(  0.02%)
                                        0.0003  0.6439  0.0009 -0.0079 -0.0014
                                       -0.3842 -0.0057  0.0086 -0.3996  0.0034
                                        0.0018  0.5269 -0.0074  0.0050  0.0076
                                        0.0007  0.0047  0.0094 -0.0089
              ( 50.00%)  -0.7071* B  15 s( 35.85%)p 1.79( 64.13%)d 0.00(  0.02%)
                                        0.0005  0.5986  0.0042 -0.0098 -0.0020
                                        0.7256 -0.0099 -0.0112  0.1869 -0.0087
                                       -0.0056  0.2817  0.0076  0.0063  0.0093
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                                     -0.0066 -0.0034  0.0077 -0.0060
1485. (0.05483) BD*( 1) B  15 - C  16
              ( 66.05%)   0.8127* B  15 s( 37.77%)p 1.65( 62.19%)d 0.00(  0.04%)
                                     -0.0012  0.6145  0.0018  0.0069  0.0010
                                     -0.5565  0.0034 -0.0173 -0.3990  0.0015
                                     -0.0123  0.3904  0.0032  0.0120  0.0138
                                     -0.0106 -0.0073  0.0053 -0.0034
              ( 33.95%)  -0.5827* C  16 s( 46.89%)p 1.13( 53.11%)d 0.00(  0.01%)
                                      0.0000  0.6845 -0.0171 -0.0050  0.0001
                                      0.5370 -0.0245 -0.0049  0.4029 -0.0194
                                     -0.0035 -0.2812  0.0163  0.0008  0.0037
                                     -0.0034 -0.0045  0.0027 -0.0010
1486. (0.04814) BD*( 1) C  16 - N  17
              ( 62.95%)   0.7934* C  16 s( 26.30%)p 2.80( 73.63%)d 0.00(  0.07%)
                                     -0.0004  0.5122  0.0236  0.0037 -0.0003
                                     -0.8032 -0.0162 -0.0108 -0.0083  0.0092
                                      0.0049 -0.3003 -0.0176 -0.0091  0.0067
                                      0.0107  0.0011  0.0214 -0.0115
              ( 37.05%)  -0.6087* N  17 s( 34.38%)p 1.91( 65.56%)d 0.00(  0.06%)
                                     -0.0001  0.5864 -0.0022 -0.0015  0.0001
                                      0.7863 -0.0066 -0.0019  0.0549 -0.0116
                                      0.0031  0.1846  0.0087 -0.0045  0.0012
                                      0.0131 -0.0012  0.0179 -0.0081
1487. (0.60501) BD*( 2) C  16 - N  17
              ( 74.06%)   0.8606* C  16 s(  0.07%)p99.99( 99.77%)d 2.47(  0.16%)
                                      0.0001  0.0253  0.0036 -0.0009  0.0004
                                     -0.2338 -0.0032 -0.0016  0.7218  0.0263
                                     -0.0108  0.6489  0.0149 -0.0030 -0.0258
                                     -0.0251 -0.0090  0.0145 -0.0061
              ( 25.94%)  -0.5093* N  17 s(  0.02%)p99.99( 99.96%)d 0.83(  0.02%)
                                      0.0000 -0.0143  0.0040 -0.0006  0.0000
                                     -0.1986 -0.0038 -0.0022  0.7039  0.0040
                                      0.0076  0.6816  0.0057  0.0065  0.0077
                                      0.0049  0.0034  0.0004  0.0094
1488. (0.05247) BD*( 1) C  16 - N  20
              ( 62.98%)   0.7936* C  16 s( 26.80%)p 2.73( 73.13%)d 0.00(  0.07%)
                                     -0.0003  0.5170  0.0259  0.0042 -0.0001
                                      0.0963  0.0178  0.0088 -0.5605 -0.0103
                                     -0.0076  0.6379  0.0143  0.0130  0.0019
                                     -0.0022 -0.0231 -0.0113  0.0068
              ( 37.02%)  -0.6085* N  20 s( 34.60%)p 1.89( 65.35%)d 0.00(  0.05%)
                                     -0.0001  0.5882 -0.0036 -0.0020  0.0001
                                      0.0229 -0.0153  0.0047  0.5448 -0.0081
                                     -0.0012 -0.5965  0.0009  0.0033 -0.0013
                                      0.0028 -0.0204 -0.0079  0.0071
1489. (0.03043) BD*( 1) N  17 - C  18
              ( 38.06%)   0.6169* N  17 s( 31.37%)p 2.19( 68.57%)d 0.00(  0.05%)
                                      0.0001 -0.5601  0.0057  0.0000 -0.0001
                                      0.4787 -0.0226  0.0035  0.5294 -0.0078
                                     -0.0015 -0.4191 -0.0062  0.0032 -0.0129
                                      0.0110  0.0158  0.0027  0.0006
              ( 61.94%)  -0.7870* C  18 s( 28.59%)p 2.50( 71.35%)d 0.00(  0.07%)
                                      0.0001 -0.5346 -0.0044 -0.0015  0.0011
                                     -0.3761  0.0019  0.0064 -0.5764 -0.0225
                                     -0.0011  0.4884  0.0260  0.0067 -0.0166
                                      0.0107  0.0163  0.0000  0.0038
1490. (0.04192) BD*( 1) N  17 - C  21
              ( 36.89%)   0.6074* N  17 s( 34.18%)p 1.92( 65.78%)d 0.00(  0.03%)
                                      0.0001 -0.5846 -0.0029 -0.0013  0.0001
                                      0.3348  0.0051 -0.0045 -0.4695 -0.0027
                                      0.0052  0.5702  0.0066 -0.0070  0.0074
                                     -0.0091  0.0141  0.0023 -0.0024
              ( 63.11%)  -0.7944* C  21 s( 25.90%)p 2.86( 74.02%)d 0.00(  0.07%)
                                      0.0002 -0.5088 -0.0080 -0.0075  0.0006
                                     -0.3843 -0.0033 -0.0051  0.5020 -0.0002
                                      0.0066 -0.5834 -0.0058 -0.0075  0.0121
                                     -0.0132  0.0184  0.0049 -0.0059
1491. (0.00978) BD*( 1) C  18 - C  19
              ( 50.03%)   0.7073* C  18 s( 37.04%)p 1.70( 62.91%)d 0.00(  0.05%)
                                      0.0000 -0.6085 -0.0095 -0.0027 -0.0007
                                     -0.4291  0.0111  0.0143  0.3778  0.0241
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                                     0.0094 -0.5484 -0.0219 -0.0041  0.0081
                                    -0.0167  0.0116 -0.0080 -0.0012
              ( 49.97%)  -0.7069* C  19 s( 37.19%)p 1.69( 62.76%)d 0.00(  0.05%)
                                     0.0000 -0.6097 -0.0092 -0.0028 -0.0006
                                     0.5697  0.0334  0.0103 -0.2598  0.0086
                                     0.0130  0.4838  0.0013 -0.0070  0.0083
                                    -0.0153  0.0146 -0.0040 -0.0036
1492. (0.28227) BD*( 2) C  18 - C  19
              ( 50.33%)   0.7095* C  18 s(  0.00%)p 1.00( 99.94%)d 0.00(  0.06%)
                                     0.0000  0.0007 -0.0023  0.0012  0.0001
                                    -0.2259  0.0043  0.0000  0.7106 -0.0159
                                     0.0003  0.6655 -0.0144  0.0008  0.0156
                                     0.0102  0.0056 -0.0009  0.0149
              ( 49.67%)  -0.7047* C  19 s(  0.00%)p 1.00( 99.94%)d 0.00(  0.06%)
                                     0.0000  0.0027 -0.0028  0.0019  0.0001
                                    -0.2352  0.0051 -0.0005  0.7109 -0.0170
                                     0.0014  0.6620 -0.0139  0.0000 -0.0099
                                    -0.0021 -0.0036 -0.0074 -0.0203
1493. (0.01214) BD*( 1) C  18 - H  63
              ( 37.80%)   0.6148* C  18 s( 34.32%)p 1.91( 65.66%)d 0.00(  0.02%)
                                    -0.0003  0.5857 -0.0077 -0.0033  0.0002
                                    -0.7890  0.0146 -0.0005 -0.1341  0.0003
                                    -0.0085 -0.1252  0.0058  0.0082  0.0036
                                     0.0043  0.0000  0.0120 -0.0068
              ( 62.20%)  -0.7886* H  63 s( 99.93%)p 0.00(  0.07%)
                                     0.9997  0.0018  0.0002  0.0252  0.0037
                                     0.0045
1494. (0.03069) BD*( 1) C  19 - N  20
              ( 62.02%)   0.7875* C  19 s( 28.42%)p 2.52( 71.51%)d 0.00(  0.07%)
                                    -0.0001  0.5331  0.0043  0.0013 -0.0012
                                     0.7774  0.0331  0.0053  0.3228  0.0004
                                    -0.0070 -0.0726  0.0095  0.0051  0.0178
                                    -0.0061 -0.0073  0.0116 -0.0109
              ( 37.98%)  -0.6163* N  20 s( 31.27%)p 2.20( 68.68%)d 0.00(  0.05%)
                                    -0.0001  0.5592 -0.0037  0.0003  0.0001
                                    -0.7108  0.0036  0.0032 -0.3916  0.0201
                                    -0.0033  0.1659 -0.0141  0.0029  0.0148
                                    -0.0045 -0.0036  0.0134 -0.0104
1495. (0.01258) BD*( 1) C  19 - H  64
              ( 37.87%)   0.6154* C  19 s( 34.33%)p 1.91( 65.65%)d 0.00(  0.02%)
                                    -0.0003  0.5858 -0.0073 -0.0033  0.0002
                                    -0.1129 -0.0021 -0.0106 -0.5674  0.0108
                                    -0.0028  0.5669 -0.0110 -0.0037  0.0022
                                    -0.0018 -0.0130 -0.0057  0.0036
              ( 62.13%)  -0.7882* H  64 s( 99.93%)p 0.00(  0.07%)
                                     0.9997  0.0019  0.0002  0.0030  0.0183
                                    -0.0182
1496. (0.04104) BD*( 1) N  20 - C  31
              ( 37.22%)   0.6101* N  20 s( 34.08%)p 1.93( 65.89%)d 0.00(  0.04%)
                                     0.0001 -0.5838 -0.0027 -0.0017  0.0002
                                    -0.6545 -0.0049  0.0078  0.1638  0.0043
                                    -0.0023 -0.4511 -0.0052  0.0056  0.0032
                                    -0.0152  0.0046 -0.0103 -0.0002
              ( 62.78%)  -0.7923* C  31 s( 26.18%)p 2.82( 73.75%)d 0.00(  0.07%)
                                     0.0002 -0.5116 -0.0082 -0.0071  0.0004
                                     0.6697  0.0030  0.0076 -0.1648 -0.0037
                                    -0.0014  0.5115  0.0015  0.0063  0.0069
                                    -0.0213  0.0037 -0.0136 -0.0005
1497. (0.03442) BD*( 1) C  21 - C  22
              ( 49.11%)   0.7008* C  21 s( 37.14%)p 1.69( 62.82%)d 0.00(  0.05%)
                                     0.0002 -0.6094  0.0012  0.0033 -0.0001
                                    -0.0162  0.0063  0.0045  0.2457 -0.0018
                                     0.0007  0.7533  0.0054 -0.0006  0.0014
                                    -0.0002 -0.0119  0.0035 -0.0176
              ( 50.89%)  -0.7133* C  22 s( 33.53%)p 1.98( 66.42%)d 0.00(  0.06%)
                                     0.0000 -0.5790 -0.0030  0.0011  0.0000
                                    -0.0120  0.0097  0.0007 -0.2101 -0.0098
                                     0.0023 -0.7872 -0.0007 -0.0016  0.0018
                                     0.0009 -0.0108  0.0026 -0.0206
1498. (0.03531) BD*( 1) C  21 - C  26
              ( 49.51%)   0.7036* C  21 s( 36.89%)p 1.71( 63.07%)d 0.00(  0.05%)
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                                     0.0002 -0.6073  0.0019  0.0025 -0.0002
                                     0.3615  0.0084  0.0040 -0.6531 -0.0045
                                    -0.0017 -0.2708  0.0021  0.0000  0.0152
                                     0.0061 -0.0106  0.0082  0.0049
              ( 50.49%)  -0.7105* C  26 s( 34.11%)p 1.93( 65.83%)d 0.00(  0.05%)
                                     0.0000 -0.5841 -0.0031  0.0005  0.0000
                                    -0.3858  0.0048  0.0013  0.6772  0.0003
                                     0.0011  0.2253  0.0121 -0.0031  0.0157
                                     0.0053 -0.0105  0.0099  0.0063
1499. (0.38598) BD*( 2) C  21 - C  26
              ( 46.03%)   0.6785* C  21 s(  0.04%)p99.99( 99.94%)d 0.56(  0.02%)
                                    -0.0002 -0.0165 -0.0091  0.0003  0.0003
                                    -0.8489  0.0014  0.0054 -0.5104  0.0067
                                     0.0051  0.1348 -0.0024 -0.0031 -0.0047
                                    -0.0029  0.0004  0.0130 -0.0003
              ( 53.97%)  -0.7346* C  26 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                     0.0000 -0.0009 -0.0057  0.0020  0.0002
                                    -0.8387  0.0097  0.0036 -0.5255  0.0027
                                    -0.0014  0.1409 -0.0020 -0.0018  0.0098
                                     0.0126  0.0052 -0.0135 -0.0036
1500. (0.02275) BD*( 1) C  22 - C  23
              ( 49.55%)   0.7039* C  22 s( 34.21%)p 1.92( 65.75%)d 0.00(  0.05%)
                                     0.0001 -0.5848 -0.0089 -0.0043 -0.0003
                                     0.3818  0.0038  0.0048 -0.4604 -0.0050
                                     0.0007  0.5473 -0.0078  0.0115  0.0122
                                    -0.0121  0.0123  0.0026 -0.0031
              ( 50.45%)  -0.7103* C  23 s( 35.86%)p 1.79( 64.08%)d 0.00(  0.06%)
                                    -0.0001 -0.5988  0.0004  0.0041  0.0003
                                    -0.3862 -0.0115  0.0045  0.4769  0.0167
                                    -0.0050 -0.5135  0.0026  0.0092  0.0134
                                    -0.0132  0.0150  0.0037 -0.0054
1501. (0.32447) BD*( 2) C  22 - C  23
              ( 51.69%)   0.7190* C  22 s(  0.02%)p99.99( 99.94%)d 1.71(  0.03%)
                                    -0.0002 -0.0062 -0.0128  0.0010  0.0006
                                    -0.8456  0.0042 -0.0024 -0.5105  0.0073
                                     0.0028  0.1537 -0.0064 -0.0038 -0.0065
                                     0.0004  0.0033  0.0172 -0.0010
              ( 48.31%)  -0.6950* C  23 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.03%)
                                     0.0000 -0.0001 -0.0045  0.0001  0.0001
                                    -0.8394  0.0021 -0.0147 -0.5229  0.0037
                                    -0.0117  0.1459  0.0003  0.0029  0.0013
                                    -0.0134 -0.0097 -0.0065  0.0038
1502. (0.03210) BD*( 1) C  22 - C  27
              ( 49.80%)   0.7057* C  22 s( 32.22%)p 2.10( 67.75%)d 0.00(  0.03%)
                                     0.0001 -0.5676  0.0058  0.0042  0.0003
                                    -0.3719 -0.0040  0.0033  0.6945  0.0166
                                    -0.0064  0.2375  0.0045  0.0009  0.0117
                                     0.0025 -0.0067  0.0096  0.0059
              ( 50.20%)  -0.7085* C  27 s( 26.68%)p 2.75( 73.27%)d 0.00(  0.06%)
                                    -0.0001 -0.5165 -0.0001  0.0014 -0.0005
                                     0.3744 -0.0052 -0.0001 -0.7310 -0.0012
                                     0.0007 -0.2409 -0.0001  0.0030  0.0156
                                     0.0057 -0.0105  0.0102  0.0090
1503. (0.01470) BD*( 1) C  23 - C  24
              ( 49.89%)   0.7064* C  23 s( 35.87%)p 1.79( 64.07%)d 0.00(  0.05%)
                                     0.0000 -0.5988 -0.0135 -0.0054 -0.0002
                                     0.3811  0.0137  0.0036 -0.6705 -0.0165
                                    -0.0022 -0.2117  0.0198  0.0137  0.0142
                                     0.0065 -0.0133  0.0091  0.0040
              ( 50.11%)  -0.7079* C  24 s( 35.96%)p 1.78( 63.97%)d 0.00(  0.07%)
                                     0.0000 -0.5996 -0.0058  0.0020  0.0002
                                    -0.3654 -0.0027  0.0084  0.6618  0.0113
                                    -0.0099  0.2588  0.0295  0.0077  0.0197
                                     0.0032 -0.0067  0.0111  0.0102
1504. (0.01740) BD*( 1) C  23 - H  67
              ( 38.93%)   0.6239* C  23 s( 28.23%)p 2.54( 71.73%)d 0.00(  0.04%)
                                    -0.0004  0.5312 -0.0109 -0.0014  0.0001
                                    -0.0058  0.0002 -0.0024 -0.2188  0.0095
                                     0.0046 -0.8179  0.0147  0.0124 -0.0002
                                     0.0002  0.0087 -0.0015  0.0168
              ( 61.07%)  -0.7815* H  67 s( 99.94%)p 0.00(  0.06%)
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                                     0.9997 -0.0017  0.0014 -0.0015  0.0058
                                     0.0227
1505. (0.01474) BD*( 1) C  24 - C  25
              ( 50.24%)   0.7088* C  24 s( 35.96%)p 1.78( 63.97%)d 0.00(  0.07%)
                                     0.0000 -0.5996 -0.0080  0.0020  0.0001
                                     0.0142  0.0136  0.0068 -0.2360 -0.0263
                                    -0.0060 -0.7633 -0.0136  0.0116  0.0014
                                    -0.0031 -0.0075  0.0015 -0.0243
              ( 49.76%)  -0.7054* C  25 s( 36.10%)p 1.77( 63.85%)d 0.00(  0.05%)
                                     0.0000 -0.6007 -0.0144 -0.0044 -0.0001
                                     0.0185  0.0138  0.0087  0.1930 -0.0170
                                    -0.0104  0.7744  0.0202  0.0033  0.0022
                                     0.0021 -0.0135  0.0033 -0.0176
1506. (0.33515) BD*( 2) C  24 - C  25
              ( 51.15%)   0.7152* C  24 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                     0.0000  0.0002  0.0031 -0.0021  0.0001
                                     0.8406 -0.0071  0.0095  0.5212 -0.0042
                                     0.0054 -0.1457  0.0013 -0.0018  0.0007
                                     0.0125  0.0084  0.0044 -0.0043
              ( 48.85%)  -0.6989* C  25 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                                     0.0001  0.0006  0.0011 -0.0012 -0.0003
                                     0.8397 -0.0082  0.0181  0.5214 -0.0050
                                     0.0106 -0.1495 -0.0003 -0.0033 -0.0059
                                    -0.0092 -0.0038  0.0092  0.0025
1507. (0.01546) BD*( 1) C  24 - H  66
              ( 39.10%)   0.6253* C  24 s( 28.03%)p 2.57( 71.94%)d 0.00(  0.03%)
                                     0.0004 -0.5293  0.0115 -0.0035 -0.0003
                                     0.3984 -0.0123  0.0025 -0.4827  0.0132
                                    -0.0020  0.5719 -0.0153  0.0022  0.0045
                                    -0.0098  0.0143 -0.0006 -0.0005
              ( 60.90%)  -0.7804* H  66 s( 99.95%)p 0.00(  0.05%)
                                    -0.9997 -0.0014 -0.0005 -0.0106  0.0132
                                    -0.0158
1508. (0.02276) BD*( 1) C  25 - C  26
              ( 50.63%)   0.7116* C  25 s( 35.74%)p 1.80( 64.20%)d 0.00(  0.06%)
                                     0.0001  0.5978 -0.0017 -0.0044 -0.0001
                                     0.3694  0.0031 -0.0060 -0.4342  0.0022
                                     0.0071  0.5626  0.0199 -0.0057 -0.0129
                                     0.0134 -0.0148 -0.0033  0.0060
              ( 49.37%)  -0.7026* C  26 s( 33.98%)p 1.94( 65.97%)d 0.00(  0.05%)
                                    -0.0002  0.5828  0.0099  0.0029  0.0001
                                    -0.3836  0.0037 -0.0077  0.4652 -0.0079
                                     0.0077 -0.5441 -0.0034  0.0000 -0.0110
                                     0.0119 -0.0127 -0.0023  0.0058
1509. (0.01723) BD*( 1) C  25 - H  65
              ( 39.19%)   0.6260* C  25 s( 28.12%)p 2.55( 71.84%)d 0.00(  0.04%)
                                     0.0004 -0.5302  0.0105  0.0004 -0.0001
                                     0.3966 -0.0066 -0.0044 -0.7080  0.0112
                                     0.0105 -0.2439  0.0108  0.0055  0.0129
                                     0.0046 -0.0083  0.0079  0.0066
              ( 60.81%)  -0.7798* H  65 s( 99.95%)p 0.00(  0.05%)
                                    -0.9997 -0.0020 -0.0013 -0.0105  0.0195
                                     0.0069
1510. (0.03221) BD*( 1) C  26 - C  29
              ( 49.95%)   0.7068* C  26 s( 31.88%)p 2.14( 68.09%)d 0.00(  0.03%)
                                     0.0001 -0.5645  0.0074  0.0031  0.0002
                                     0.0045  0.0027  0.0007 -0.2195 -0.0065
                                     0.0004 -0.7952 -0.0162  0.0049  0.0013
                                     0.0000 -0.0072  0.0015 -0.0161
              ( 50.05%)  -0.7075* C  29 s( 26.68%)p 2.75( 73.27%)d 0.00(  0.06%)
                                    -0.0001 -0.5165 -0.0016  0.0017  0.0001
                                    -0.0141 -0.0025  0.0022  0.2394  0.0010
                                    -0.0018  0.8217 -0.0018 -0.0030  0.0001
                                     0.0005 -0.0113  0.0015 -0.0206
1511. (0.01812) BD*( 1) C  27 - C  28
              ( 49.51%)   0.7037* C  27 s( 25.54%)p 2.91( 74.42%)d 0.00(  0.04%)
                                     0.0001 -0.5053  0.0112 -0.0022  0.0001
                                     0.5593 -0.0005  0.0003  0.6556  0.0122
                                     0.0041 -0.0376 -0.0039 -0.0008 -0.0172
                                     0.0017  0.0010  0.0006  0.0104
              ( 50.49%)  -0.7105* C  28 s( 29.27%)p 2.41( 70.68%)d 0.00(  0.04%)
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                                    -0.0004 -0.5407  0.0193  0.0030 -0.0001
                                    -0.5458 -0.0107  0.0077 -0.6389 -0.0071
                                     0.0132  0.0176  0.0006 -0.0013 -0.0179
                                     0.0005  0.0007  0.0031  0.0107
1512. (0.01403) BD*( 1) C  27 - C  62
              ( 48.57%)   0.6969* C  27 s( 26.93%)p 2.71( 73.03%)d 0.00(  0.04%)
                                    -0.0001  0.5188 -0.0115  0.0033 -0.0002
                                     0.3401  0.0136  0.0031  0.0651 -0.0020
                                    -0.0012 -0.7811  0.0053 -0.0039  0.0016
                                    -0.0112 -0.0022  0.0017  0.0153
              ( 51.43%)  -0.7172* C  62 s( 28.50%)p 2.51( 71.45%)d 0.00(  0.05%)
                                     0.0003  0.5334 -0.0218 -0.0029  0.0000
                                    -0.3602 -0.0039  0.0095 -0.0533 -0.0064
                                     0.0003  0.7625  0.0130 -0.0123  0.0009
                                    -0.0153 -0.0027  0.0038  0.0157
1513. (0.02449) BD*( 1) C  27 - H  84
              ( 38.38%)   0.6195* C  27 s( 20.90%)p 3.78( 79.05%)d 0.00(  0.05%)
                                     0.0002 -0.4567 -0.0204  0.0043  0.0001
                                    -0.6559  0.0047  0.0021  0.1755 -0.0063
                                     0.0063 -0.5737  0.0132  0.0056  0.0050
                                    -0.0190  0.0051 -0.0092 -0.0039
              ( 61.62%)  -0.7850* H  84 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0050 -0.0007  0.0169 -0.0024
                                     0.0125
1514. (0.00804) BD*( 1) C  28 - H  90
              ( 39.23%)   0.6264* C  28 s( 23.20%)p 3.31( 76.76%)d 0.00(  0.04%)
                                    -0.0002  0.4816  0.0056  0.0024  0.0001
                                     0.3911 -0.0046 -0.0039 -0.7480  0.0050
                                    -0.0078 -0.2347  0.0020  0.0009 -0.0144
                                    -0.0042  0.0079 -0.0098 -0.0076
              ( 60.77%)  -0.7795* H  90 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0016  0.0002 -0.0112  0.0159
                                     0.0062
1515. (0.00798) BD*( 1) C  28 - H  91
              ( 39.54%)   0.6288* C  28 s( 23.87%)p 3.19( 76.08%)d 0.00(  0.05%)
                                     0.0000  0.4885  0.0040  0.0014 -0.0001
                                    -0.3302  0.0010 -0.0058 -0.1091 -0.0013
                                    -0.0084  0.7999 -0.0030 -0.0005 -0.0004
                                    -0.0132 -0.0049  0.0032  0.0169
              ( 60.46%)  -0.7776* H  91 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0016  0.0000  0.0060  0.0017
                                    -0.0197
1516. (0.01047) BD*( 1) C  28 - H  92
              ( 39.32%)   0.6270* C  28 s( 23.66%)p 3.23( 76.30%)d 0.00(  0.05%)
                                     0.0000  0.4863  0.0077 -0.0005  0.0000
                                    -0.6627 -0.0002 -0.0075  0.1397 -0.0033
                                    -0.0065 -0.5516  0.0033 -0.0004 -0.0055
                                     0.0170 -0.0029  0.0109  0.0023
              ( 60.68%)  -0.7790* H  92 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0023  0.0002  0.0155 -0.0051
                                     0.0144
1517. (0.01761) BD*( 1) C  29 - C  30
              ( 49.31%)   0.7022* C  29 s( 26.01%)p 2.84( 73.95%)d 0.00(  0.04%)
                                     0.0001 -0.5098  0.0125 -0.0007  0.0000
                                     0.8057  0.0033  0.0026 -0.0250  0.0086
                                    -0.0004 -0.2992 -0.0115 -0.0030  0.0012
                                     0.0098 -0.0003 -0.0155  0.0063
              ( 50.69%)  -0.7120* C  30 s( 29.30%)p 2.41( 70.65%)d 0.00(  0.05%)
                                    -0.0003 -0.5410  0.0190  0.0027 -0.0001
                                    -0.7841 -0.0125  0.0134  0.0260  0.0014
                                     0.0007  0.3011  0.0002 -0.0070  0.0006
                                     0.0124 -0.0001 -0.0161  0.0065
1518. (0.01761) BD*( 1) C  29 - C  61
              ( 48.72%)   0.6980* C  29 s( 26.46%)p 2.78( 73.50%)d 0.00(  0.04%)
                                     0.0001 -0.5143  0.0111 -0.0012 -0.0001
                                    -0.3898 -0.0116 -0.0009 -0.7555  0.0018
                                    -0.0055 -0.1098 -0.0075 -0.0042 -0.0130
                                    -0.0013 -0.0030  0.0098  0.0089
              ( 51.28%)  -0.7161* C  61 s( 28.85%)p 2.46( 71.10%)d 0.00(  0.05%)
                                    -0.0003 -0.5370  0.0135 -0.0007  0.0005
                                     0.3908  0.0054 -0.0080  0.7377  0.0078
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                                    -0.0073  0.1179 -0.0041 -0.0017 -0.0154
                                    -0.0026 -0.0043  0.0098  0.0100
1519. (0.02465) BD*( 1) C  29 - H  83
              ( 38.95%)   0.6241* C  29 s( 20.90%)p 3.78( 79.05%)d 0.00(  0.05%)
                                     0.0002 -0.4567 -0.0201  0.0004 -0.0001
                                    -0.4447  0.0057  0.0051  0.6083 -0.0122
                                    -0.0052 -0.4717  0.0062 -0.0050  0.0137
                                    -0.0105  0.0147  0.0046  0.0018
              ( 61.05%)  -0.7813* H  83 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0054 -0.0001  0.0113 -0.0145
                                     0.0104
1520. (0.00762) BD*( 1) C  30 - H  93
              ( 39.26%)   0.6265* C  30 s( 23.29%)p 3.29( 76.67%)d 0.00(  0.04%)
                                     0.0001 -0.4826 -0.0052 -0.0019 -0.0002
                                    -0.0011  0.0026  0.0077 -0.2021  0.0017
                                     0.0005 -0.8519  0.0056 -0.0047  0.0000
                                    -0.0001 -0.0081  0.0019 -0.0193
              ( 60.74%)  -0.7794* H  93 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0015 -0.0002  0.0020  0.0050
                                     0.0203
1521. (0.01056) BD*( 1) C  30 - H  94
              ( 39.34%)   0.6272* C  30 s( 23.75%)p 3.21( 76.20%)d 0.00(  0.05%)
                                     0.0000 -0.4873 -0.0067  0.0002  0.0001
                                     0.4764  0.0046  0.0087 -0.6003  0.0031
                                    -0.0010  0.4178 -0.0031 -0.0025  0.0138
                                    -0.0106  0.0112  0.0039  0.0031
              ( 60.66%)  -0.7789* H  94 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0022 -0.0002 -0.0107  0.0148
                                    -0.0113
1522. (0.00687) BD*( 1) C  30 - H  95
              ( 39.27%)   0.6267* C  30 s( 23.66%)p 3.22( 76.29%)d 0.00(  0.05%)
                                     0.0001 -0.4864 -0.0049 -0.0014  0.0001
                                     0.3962  0.0009  0.0082  0.7729 -0.0056
                                     0.0006  0.0916 -0.0009 -0.0042 -0.0150
                                    -0.0031 -0.0031  0.0112  0.0091
              ( 60.73%)  -0.7793* H  95 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0012 -0.0001 -0.0092 -0.0184
                                    -0.0025
1523. (0.03513) BD*( 1) C  31 - C  32
              ( 49.39%)   0.7028* C  31 s( 36.78%)p 1.72( 63.17%)d 0.00(  0.05%)
                                     0.0002 -0.6065  0.0017  0.0032 -0.0001
                                    -0.0389 -0.0034 -0.0005 -0.4016  0.0020
                                     0.0015 -0.6847 -0.0088 -0.0028  0.0012
                                    -0.0011 -0.0166  0.0036 -0.0135
              ( 50.61%)  -0.7114* C  32 s( 33.82%)p 1.96( 66.13%)d 0.00(  0.05%)
                                     0.0000 -0.5815 -0.0025  0.0007  0.0000
                                     0.0788 -0.0101  0.0023  0.3802  0.0088
                                    -0.0001  0.7143 -0.0021 -0.0014  0.0004
                                    -0.0025 -0.0176  0.0042 -0.0140
1524. (0.03523) BD*( 1) C  31 - C  36
              ( 49.27%)   0.7020* C  31 s( 36.98%)p 1.70( 62.97%)d 0.00(  0.05%)
                                     0.0002 -0.6081  0.0016  0.0025 -0.0001
                                    -0.5173 -0.0061  0.0000  0.5489  0.0054
                                     0.0031  0.2464 -0.0054 -0.0025  0.0169
                                     0.0061 -0.0095  0.0022  0.0070
              ( 50.73%)  -0.7122* C  36 s( 33.78%)p 1.96( 66.16%)d 0.00(  0.05%)
                                     0.0000 -0.5812 -0.0025  0.0001  0.0000
                                     0.5450 -0.0036  0.0022 -0.5690 -0.0023
                                     0.0011 -0.2015 -0.0133  0.0006  0.0186
                                     0.0066 -0.0093  0.0008  0.0077
1525. (0.37263) BD*( 2) C  31 - C  36
              ( 45.69%)   0.6759* C  31 s(  0.01%)p99.99( 99.97%)d 1.31(  0.02%)
                                    -0.0002 -0.0082 -0.0087  0.0009  0.0001
                                    -0.5306  0.0061  0.0063 -0.7140  0.0026
                                     0.0042  0.4562 -0.0007 -0.0033 -0.0013
                                     0.0047 -0.0046 -0.0119 -0.0012
              ( 54.31%)  -0.7370* C  36 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                     0.0000 -0.0004 -0.0057  0.0010  0.0001
                                    -0.5517  0.0041 -0.0008 -0.6923  0.0101
                                     0.0043  0.4644 -0.0046 -0.0005 -0.0017
                                    -0.0118 -0.0024  0.0155  0.0107
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1526. (0.02267) BD*( 1) C  32 - C  33
              ( 49.44%)   0.7032* C  32 s( 34.05%)p 1.94( 65.90%)d 0.00(  0.05%)
                                        0.0001 -0.5834 -0.0094 -0.0040 -0.0001
                                       -0.6245 -0.0001 -0.0038  0.1621  0.0065
                                       -0.0023 -0.4925  0.0078 -0.0093  0.0081
                                       -0.0169  0.0031 -0.0103 -0.0005
              ( 50.56%)  -0.7110* C  33 s( 35.75%)p 1.80( 64.19%)d 0.00(  0.06%)
                                       -0.0001 -0.5979  0.0011  0.0044  0.0001
                                        0.6298  0.0154 -0.0076 -0.1843 -0.0134
                                        0.0007  0.4591 -0.0018 -0.0081  0.0085
                                       -0.0198  0.0030 -0.0117 -0.0013
1527. (0.34032) BD*( 2) C  32 - C  33
              ( 51.62%)   0.7184* C  32 s(  0.01%)p 1.00( 99.96%)d 0.00(  0.03%)
                                        0.0001  0.0002  0.0071 -0.0021 -0.0001
                                        0.5350 -0.0046 -0.0012  0.7197 -0.0022
                                        0.0042 -0.4419  0.0039  0.0014  0.0053
                                       -0.0052  0.0062  0.0150 -0.0017
              ( 48.38%)  -0.6956* C  33 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                        0.0001  0.0016  0.0012 -0.0001 -0.0001
                                        0.5376 -0.0028  0.0092  0.7132 -0.0032
                                        0.0113 -0.4491  0.0015 -0.0089 -0.0083
                                       -0.0035 -0.0097 -0.0037  0.0113
1528. (0.03229) BD*( 1) C  32 - C  37
              ( 49.77%)   0.7055* C  32 s( 32.10%)p 2.11( 67.87%)d 0.00(  0.03%)
                                        0.0001 -0.5665  0.0064  0.0038  0.0000
                                        0.5628  0.0103 -0.0042 -0.5572 -0.0122
                                        0.0048 -0.2264 -0.0063  0.0002  0.0144
                                        0.0047 -0.0061 -0.0010  0.0064
              ( 50.23%)  -0.7087* C  37 s( 26.54%)p 2.77( 73.40%)d 0.00(  0.06%)
                                       -0.0001 -0.5152 -0.0012  0.0021  0.0001
                                       -0.5819  0.0019  0.0024  0.5808 -0.0006
                                       -0.0011  0.2409  0.0016 -0.0035  0.0189
                                        0.0080 -0.0079  0.0002  0.0090
1529. (0.01475) BD*( 1) C  33 - C  34
              ( 49.78%)   0.7056* C  33 s( 36.06%)p 1.77( 63.89%)d 0.00(  0.05%)
                                        0.0000 -0.6003 -0.0142 -0.0045  0.0000
                                       -0.5534 -0.0226 -0.0069  0.5416  0.0063
                                       -0.0020  0.1955 -0.0178 -0.0118  0.0170
                                        0.0080 -0.0113  0.0022  0.0056
              ( 50.22%)  -0.7086* C  34 s( 35.89%)p 1.78( 64.04%)d 0.00(  0.07%)
                                        0.0000 -0.5990 -0.0074  0.0018  0.0001
                                        0.5213 -0.0002 -0.0098 -0.5587 -0.0181
                                        0.0052 -0.2351 -0.0270 -0.0075  0.0221
                                        0.0044 -0.0059 -0.0021  0.0108
1530. (0.01721) BD*( 1) C  33 - H  70
              ( 39.08%)   0.6251* C  33 s( 28.16%)p 2.55( 71.80%)d 0.00(  0.04%)
                                        0.0004 -0.5306  0.0109  0.0005 -0.0001
                                       -0.0816 -0.0035 -0.0002 -0.4036  0.0098
                                        0.0078 -0.7403  0.0129  0.0104 -0.0010
                                       -0.0026 -0.0140  0.0038 -0.0120
              ( 60.92%)  -0.7805* H  70 s( 99.95%)p 0.00(  0.05%)
                                       -0.9997 -0.0019 -0.0013  0.0021  0.0114
                                        0.0202
1531. (0.01478) BD*( 1) C  34 - C  35
              ( 50.12%)   0.7080* C  34 s( 36.02%)p 1.77( 63.92%)d 0.00(  0.06%)
                                        0.0000  0.6001  0.0067 -0.0022 -0.0002
                                       -0.0528  0.0196  0.0070 -0.4018 -0.0227
                                       -0.0036 -0.6883 -0.0117  0.0110  0.0021
                                        0.0078  0.0170 -0.0027  0.0169
              ( 49.88%)  -0.7062* C  35 s( 35.99%)p 1.78( 63.96%)d 0.00(  0.05%)
                                        0.0000  0.5997  0.0141  0.0044  0.0001
                                        0.0989  0.0230  0.0088  0.3787 -0.0068
                                       -0.0087  0.6967  0.0182  0.0056 -0.0012
                                       -0.0001  0.0182 -0.0056  0.0119
1532. (0.33303) BD*( 2) C  34 - C  35
              ( 50.89%)   0.7134* C  34 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                        0.0000 -0.0020  0.0008 -0.0041 -0.0002
                                        0.5464 -0.0043  0.0015  0.7032 -0.0061
                                        0.0062 -0.4543  0.0042 -0.0038 -0.0066
                                       -0.0054 -0.0090 -0.0019  0.0108
              ( 49.11%)  -0.7008* C  35 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.02%)
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                                     0.0000 -0.0028 -0.0012 -0.0004 -0.0007
                                     0.5503 -0.0039  0.0071  0.6993 -0.0056
                                     0.0123 -0.4556  0.0037 -0.0088  0.0026
                                     0.0080  0.0007 -0.0107 -0.0078
1533. (0.01550) BD*( 1) C  34 - H  69
              ( 38.99%)   0.6244* C  34 s( 28.04%)p 2.56( 71.92%)d 0.00(  0.03%)
                                     0.0004 -0.5294  0.0119 -0.0035 -0.0003
                                    -0.6523  0.0173 -0.0025  0.1740 -0.0054
                                     0.0021 -0.5127  0.0149 -0.0043  0.0013
                                    -0.0134  0.0081 -0.0086  0.0004
              ( 61.01%)  -0.7811* H  69 s( 99.95%)p 0.00(  0.05%)
                                    -0.9997 -0.0014 -0.0005  0.0178 -0.0047
                                     0.0142
1534. (0.02305) BD*( 1) C  35 - C  36
              ( 50.57%)   0.7111* C  35 s( 35.77%)p 1.79( 64.16%)d 0.00(  0.06%)
                                     0.0001  0.5981 -0.0014 -0.0046 -0.0001
                                    -0.6018 -0.0037  0.0070  0.1453 -0.0067
                                    -0.0042 -0.5078 -0.0186  0.0049 -0.0082
                                     0.0202 -0.0033  0.0114  0.0020
              ( 49.43%)  -0.7031* C  36 s( 34.00%)p 1.94( 65.95%)d 0.00(  0.05%)
                                    -0.0001  0.5830  0.0097  0.0032  0.0001
                                     0.6250 -0.0061  0.0075 -0.1702  0.0068
                                    -0.0074  0.4895  0.0045  0.0014 -0.0066
                                     0.0177 -0.0026  0.0094  0.0028
1535. (0.01717) BD*( 1) C  35 - H  68
              ( 38.96%)   0.6242* C  35 s( 28.21%)p 2.54( 71.76%)d 0.00(  0.04%)
                                     0.0004 -0.5310  0.0105  0.0002 -0.0001
                                    -0.5693  0.0071  0.0068  0.5878 -0.0130
                                    -0.0069  0.2180 -0.0083 -0.0055  0.0152
                                     0.0057 -0.0065  0.0008  0.0073
              ( 61.04%)  -0.7813* H  68 s( 99.95%)p 0.00(  0.05%)
                                    -0.9997  0.0019 -0.0015  0.0154 -0.0159
                                    -0.0066
1536. (0.03217) BD*( 1) C  36 - C  39
              ( 49.62%)   0.7044* C  36 s( 32.18%)p 2.11( 67.79%)d 0.00(  0.03%)
                                     0.0001 -0.5672  0.0067  0.0038  0.0001
                                     0.0846  0.0002 -0.0016  0.4088  0.0113
                                    -0.0023  0.7094  0.0143 -0.0049 -0.0009
                                    -0.0040 -0.0133  0.0031 -0.0101
              ( 50.38%)  -0.7098* C  39 s( 26.43%)p 2.78( 73.51%)d 0.00(  0.06%)
                                    -0.0001 -0.5141 -0.0010  0.0021  0.0002
                                    -0.0840  0.0010 -0.0001 -0.4367 -0.0029
                                     0.0041 -0.7330  0.0018  0.0024 -0.0019
                                    -0.0031 -0.0177  0.0054 -0.0146
1537. (0.01669) BD*( 1) C  37 - C  38
              ( 49.23%)   0.7017* C  37 s( 26.24%)p 2.81( 73.73%)d 0.00(  0.04%)
                                     0.0001 -0.5120  0.0130 -0.0007  0.0000
                                     0.2983  0.0144  0.0026  0.1711  0.0027
                                    -0.0009 -0.7866  0.0000 -0.0023 -0.0018
                                     0.0100  0.0067 -0.0012 -0.0151
              ( 50.77%)  -0.7125* C  38 s( 29.30%)p 2.41( 70.66%)d 0.00(  0.05%)
                                    -0.0003 -0.5409  0.0191  0.0022 -0.0001
                                    -0.3080 -0.0004  0.0074 -0.1553 -0.0041
                                     0.0026  0.7663  0.0125 -0.0130 -0.0027
                                     0.0126  0.0067 -0.0021 -0.0157
1538. (0.01793) BD*( 1) C  37 - C  55
              ( 48.57%)   0.6969* C  37 s( 26.40%)p 2.79( 73.56%)d 0.00(  0.03%)
                                     0.0001 -0.5137  0.0103 -0.0015 -0.0001
                                    -0.3214  0.0052  0.0016 -0.7940 -0.0075
                                    -0.0068  0.0400  0.0084 -0.0028 -0.0118
                                     0.0009  0.0010  0.0108  0.0095
              ( 51.43%)  -0.7172* C  55 s( 28.68%)p 2.48( 71.27%)d 0.00(  0.05%)
                                    -0.0004 -0.5354  0.0131 -0.0008  0.0005
                                     0.3100  0.0081 -0.0025  0.7838  0.0066
                                    -0.0090 -0.0450 -0.0031  0.0042 -0.0125
                                     0.0009  0.0026  0.0133  0.0107
1539. (0.02520) BD*( 1) C  37 - H  85
              ( 38.85%)   0.6233* C  37 s( 20.87%)p 3.79( 79.08%)d 0.00(  0.05%)
                                    -0.0002  0.4564  0.0202 -0.0004  0.0001
                                    -0.6842  0.0102 -0.0026 -0.0463  0.0035
                                     0.0031 -0.5659  0.0096  0.0078  0.0018
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                                     0.0195  0.0016  0.0118  0.0025
             ( 61.15%)  -0.7820* H  85 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0055  0.0003  0.0160  0.0013
                                     0.0141
1540. (0.00720) BD*( 1) C  38 - H 105
             ( 39.14%)   0.6256* C  38 s( 23.26%)p 3.30( 76.70%)d 0.00(  0.04%)
                                     0.0001 -0.4823 -0.0050 -0.0014 -0.0002
                                     0.6347 -0.0039  0.0046 -0.5690  0.0053
                                     0.0016 -0.2004 -0.0007 -0.0077  0.0169
                                     0.0055 -0.0062 -0.0016  0.0093
             ( 60.86%)  -0.7801* H 105 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0013 -0.0002 -0.0151  0.0144
                                     0.0031
1541. (0.00679) BD*( 1) C  38 - H 106
             ( 39.17%)   0.6258* C  38 s( 23.69%)p 3.22( 76.26%)d 0.00(  0.04%)
                                     0.0001 -0.4867 -0.0057 -0.0014  0.0001
                                     0.3371 -0.0018  0.0046  0.8043 -0.0049
                                     0.0022 -0.0449 -0.0034 -0.0073 -0.0122
                                    -0.0001  0.0020  0.0124  0.0117
             ( 60.83%)  -0.7800* H 106 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0012 -0.0001 -0.0076 -0.0195
                                     0.0007
1542. (0.01082) BD*( 1) C  38 - H 107
             ( 39.43%)   0.6280* C  38 s( 23.75%)p 3.21( 76.20%)d 0.00(  0.05%)
                                     0.0000 -0.4873 -0.0061  0.0002  0.0001
                                    -0.6228  0.0046  0.0024 -0.0677  0.0027
                                     0.0014 -0.6078 -0.0039 -0.0086 -0.0015
                                    -0.0190 -0.0026 -0.0083 -0.0042
             ( 60.57%)  -0.7782* H 107 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0023 -0.0002  0.0158  0.0015
                                     0.0142
1543. (0.01773) BD*( 1) C  39 - C  40
             ( 49.31%)   0.7022* C  39 s( 25.93%)p 2.85( 74.03%)d 0.00(  0.04%)
                                     0.0001 -0.5091  0.0127 -0.0008  0.0000
                                     0.1679  0.0122  0.0013  0.8291  0.0066
                                     0.0029 -0.1563  0.0056  0.0017 -0.0059
                                     0.0010  0.0074  0.0154  0.0076
             ( 50.69%)  -0.7120* C  40 s( 29.25%)p 2.42( 70.71%)d 0.00(  0.05%)
                                    -0.0003 -0.5405  0.0192  0.0027 -0.0001
                                    -0.1631 -0.0001  0.0048 -0.8120 -0.0118
                                     0.0144  0.1443  0.0058 -0.0009 -0.0074
                                     0.0012  0.0062  0.0163  0.0097
1544. (0.01637) BD*( 1) C  39 - C  56
             ( 48.43%)   0.6959* C  39 s( 26.76%)p 2.74( 73.21%)d 0.00(  0.03%)
                                     0.0001 -0.5172  0.0107 -0.0016 -0.0001
                                    -0.6945  0.0043 -0.0029 -0.0842 -0.0075
                                     0.0041  0.4924  0.0115  0.0055 -0.0029
                                     0.0144  0.0013 -0.0107  0.0012
             ( 51.57%)  -0.7181* C  56 s( 28.64%)p 2.49( 71.31%)d 0.00(  0.05%)
                                    -0.0003 -0.5350  0.0137  0.0009  0.0005
                                     0.6749  0.0104 -0.0077  0.0911  0.0043
                                    -0.0040 -0.4991 -0.0006  0.0072 -0.0036
                                     0.0176  0.0028 -0.0117 -0.0006
1545. (0.02379) BD*( 1) C  39 - H  86
             ( 38.67%)   0.6218* C  39 s( 20.93%)p 3.78( 79.02%)d 0.00(  0.05%)
                                    -0.0002  0.4570  0.0204 -0.0005  0.0001
                                    -0.6937  0.0148  0.0011  0.3371 -0.0045
                                    -0.0086 -0.4416  0.0045 -0.0041 -0.0119
                                     0.0152 -0.0071  0.0093 -0.0035
             ( 61.33%)  -0.7831* H  86 s( 99.95%)p 0.00(  0.05%)
                                     0.9998  0.0050  0.0003  0.0161 -0.0093
                                     0.0107
1546. (0.00750) BD*( 1) C  40 - H  99
             ( 39.13%)   0.6255* C  40 s( 23.33%)p 3.28( 76.62%)d 0.00(  0.04%)
                                     0.0002 -0.4830 -0.0052 -0.0020 -0.0001
                                     0.1246 -0.0003  0.0030  0.4299 -0.0014
                                     0.0085  0.7522 -0.0064 -0.0003 -0.0022
                                    -0.0044 -0.0157  0.0032 -0.0126
             ( 60.87%)  -0.7802* H  99 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0015 -0.0002 -0.0026 -0.0085
                                    -0.0190
```

```
1547. (0.01046) BD*( 1) C  40 - H 100
              ( 39.41%)   0.6278* C  40 s( 23.74%)p 3.21( 76.21%)d 0.00(  0.05%)
                                        0.0000 -0.4872 -0.0070  0.0002  0.0001
                                       -0.6620  0.0040  0.0009  0.3821  0.0043
                                        0.0090 -0.4216 -0.0002 -0.0023  0.0130
                                       -0.0130  0.0075 -0.0076  0.0021
              ( 60.59%)  -0.7784* H 100 s( 99.95%)p 0.00(  0.05%)
                                       -0.9998 -0.0023 -0.0002  0.0169 -0.0084
                                        0.0106
1548. (0.00695) BD*( 1) C  40 - H 101
              ( 39.32%)   0.6271* C  40 s( 23.68%)p 3.22( 76.28%)d 0.00(  0.05%)
                                       -0.0001  0.4866  0.0049  0.0013 -0.0001
                                       -0.7204  0.0044 -0.0028 -0.0929 -0.0021
                                       -0.0090  0.4848 -0.0023  0.0007  0.0031
                                       -0.0160 -0.0020  0.0134  0.0006
              ( 60.68%)  -0.7790* H 101 s( 99.96%)p 0.00(  0.04%)
                                        0.9998  0.0013  0.0001  0.0172  0.0018
                                       -0.0115
1549. (0.02999) BD*( 1) C  41 - C  42
              ( 55.48%)   0.7449* C  41 s( 37.96%)p 1.30( 49.31%)d 0.34( 12.73%)
                                        0.0000 -0.6133 -0.0553 -0.0197 -0.0027
                                        0.1738 -0.0779  0.0533  0.3260  0.0165
                                       -0.0382  0.5291 -0.2482  0.0670 -0.1555
                                        0.0408 -0.2973 -0.0180 -0.1130
              ( 44.52%)  -0.6672* C  42 s( 33.58%)p 1.98( 66.37%)d 0.00(  0.05%)
                                        0.0000 -0.5794 -0.0030  0.0010  0.0000
                                       -0.1977 -0.0101  0.0001 -0.3551  0.0092
                                       -0.0019 -0.7059 -0.0035  0.0009 -0.0035
                                       -0.0108 -0.0139  0.0024 -0.0147
1550. (0.03084) BD*( 1) C  41 - C  46
              ( 56.24%)   0.7499* C  41 s( 36.17%)p 1.39( 50.23%)d 0.38( 13.60%)
                                       -0.0003  0.5978 -0.0609 -0.0258 -0.0025
                                        0.4202 -0.0918  0.0612 -0.3387  0.0307
                                       -0.0408  0.3585 -0.2513  0.0670 -0.1684
                                        0.0685 -0.3050 -0.0176 -0.0983
              ( 43.76%)  -0.6615* C  46 s( 34.19%)p 1.92( 65.76%)d 0.00(  0.05%)
                                        0.0000  0.5847  0.0020 -0.0002  0.0001
                                       -0.4969  0.0013  0.0017  0.3954 -0.0085
                                        0.0026 -0.5041 -0.0105  0.0009 -0.0112
                                        0.0162 -0.0106  0.0022  0.0038
1551. (0.37132) BD*( 2) C  41 - C  46
              ( 47.25%)   0.6874* C  41 s(  0.04%)p99.99( 98.66%)d31.71(  1.30%)
                                        0.0001  0.0118 -0.0141 -0.0085 -0.0011
                                       -0.8228 -0.0283  0.0244 -0.3815  0.0045
                                       -0.0080  0.3956 -0.0759  0.0186 -0.0462
                                        0.0154 -0.0984 -0.0174 -0.0260
              ( 52.75%)  -0.7263* C  46 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                        0.0000 -0.0021  0.0037 -0.0023  0.0000
                                       -0.7900  0.0074  0.0041 -0.4143  0.0014
                                        0.0003  0.4514 -0.0046  0.0002  0.0022
                                        0.0093  0.0084  0.0097 -0.0141
1552. (0.02303) BD*( 1) C  42 - C  43
              ( 49.61%)   0.7043* C  42 s( 34.02%)p 1.94( 65.93%)d 0.00(  0.05%)
                                        0.0001 -0.5832 -0.0088 -0.0050 -0.0002
                                       -0.2753 -0.0041 -0.0005  0.7415 -0.0016
                                        0.0070  0.1828 -0.0102  0.0089  0.0136
                                        0.0013 -0.0067  0.0129  0.0084
              ( 50.39%)  -0.7099* C  43 s( 35.87%)p 1.79( 64.06%)d 0.00(  0.06%)
                                       -0.0001 -0.5989  0.0004  0.0039  0.0003
                                        0.3007  0.0136 -0.0026 -0.7243 -0.0129
                                        0.0092 -0.1581  0.0100  0.0053  0.0146
                                        0.0012 -0.0090  0.0152  0.0090
1553. (0.33091) BD*( 2) C  42 - C  43
              ( 52.17%)   0.7223* C  42 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                       -0.0002  0.0002 -0.0028  0.0010  0.0001
                                        0.8064 -0.0066  0.0027  0.4056 -0.0017
                                       -0.0021 -0.4299  0.0017 -0.0012 -0.0069
                                       -0.0004  0.0089  0.0148 -0.0045
              ( 47.83%)  -0.6916* C  43 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                        0.0000  0.0023  0.0003 -0.0005  0.0002
                                        0.7924 -0.0040  0.0130  0.4229 -0.0035
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                                     0.0087 -0.4389  0.0043 -0.0083  0.0107
                                     0.0088 -0.0018 -0.0073 -0.0083
1554. (0.03204) BD*( 1) C  42 - C  47
              ( 49.40%)   0.7028* C  42 s( 32.37%)p 2.09( 67.60%)d 0.00(  0.03%)
                                     0.0001 -0.5689  0.0064  0.0048  0.0002
                                     0.4840  0.0068 -0.0034 -0.3985 -0.0093
                                     0.0061  0.5316  0.0132 -0.0034  0.0092
                                    -0.0114  0.0093  0.0001 -0.0027
              ( 50.60%)  -0.7114* C  47 s( 26.33%)p 2.80( 73.61%)d 0.00(  0.06%)
                                    -0.0002 -0.5132  0.0005 -0.0010 -0.0007
                                    -0.4936  0.0042  0.0002  0.4257 -0.0009
                                     0.0034 -0.5579 -0.0015 -0.0008  0.0116
                                    -0.0157  0.0134 -0.0027 -0.0026
1555. (0.01506) BD*( 1) C  43 - C  44
              ( 49.93%)   0.7066* C  43 s( 35.86%)p 1.79( 64.08%)d 0.00(  0.05%)
                                     0.0000  0.5987  0.0137  0.0045  0.0002
                                     0.4855  0.0113  0.0009 -0.4007 -0.0269
                                    -0.0107  0.4934 -0.0064 -0.0094 -0.0091
                                     0.0170 -0.0093  0.0036  0.0064
              ( 50.07%)  -0.7076* C  44 s( 35.97%)p 1.78( 63.96%)d 0.00(  0.07%)
                                     0.0000  0.5997  0.0065 -0.0023 -0.0001
                                    -0.4876 -0.0109  0.0078  0.3579 -0.0108
                                    -0.0123 -0.5220 -0.0287 -0.0016 -0.0159
                                     0.0157 -0.0125  0.0004 -0.0005
1556. (0.01779) BD*( 1) C  43 - H  75
              ( 38.93%)   0.6239* C  43 s( 28.23%)p 2.54( 71.73%)d 0.00(  0.04%)
                                    -0.0004  0.5312 -0.0110 -0.0007  0.0001
                                    -0.2119  0.0050  0.0050 -0.3668  0.0028
                                     0.0041 -0.7331  0.0148  0.0114  0.0034
                                     0.0074  0.0121 -0.0022  0.0121
              ( 61.07%)  -0.7815* H  75 s( 99.94%)p 0.00(  0.06%)
                                     0.9997 -0.0021  0.0014  0.0069  0.0098
                                     0.0202
1557. (0.01496) BD*( 1) C  44 - C  45
              ( 50.21%)   0.7086* C  44 s( 36.00%)p 1.78( 63.94%)d 0.00(  0.07%)
                                     0.0000  0.5999  0.0077 -0.0018 -0.0001
                                     0.2211  0.0194  0.0052  0.3173 -0.0121
                                    -0.0121  0.6989  0.0237 -0.0060  0.0028
                                     0.0082  0.0189 -0.0057  0.0138
              ( 49.79%)  -0.7056* C  45 s( 36.09%)p 1.77( 63.86%)d 0.00(  0.05%)
                                     0.0000  0.6005  0.0145  0.0043  0.0000
                                    -0.1901  0.0105  0.0087 -0.3628 -0.0269
                                    -0.0111 -0.6854 -0.0074  0.0027  0.0029
                                     0.0122  0.0110 -0.0004  0.0153
1558. (0.33468) BD*( 2) C  44 - C  45
              ( 51.09%)   0.7148* C  44 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                     0.0000  0.0020  0.0000  0.0013  0.0002
                                     0.7891 -0.0075  0.0086  0.4240 -0.0036
                                     0.0035 -0.4439  0.0042 -0.0045  0.0088
                                     0.0092 -0.0004 -0.0054 -0.0083
              ( 48.91%)  -0.6994* C  45 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                                     0.0000  0.0006  0.0004  0.0008  0.0003
                                     0.7888 -0.0079  0.0174  0.4249 -0.0044
                                     0.0092 -0.4432  0.0044 -0.0094 -0.0024
                                    -0.0065 -0.0058 -0.0069  0.0101
1559. (0.01582) BD*( 1) C  44 - H  74
              ( 39.13%)   0.6255* C  44 s( 27.98%)p 2.57( 71.99%)d 0.00(  0.03%)
                                    -0.0004  0.5288 -0.0120  0.0037  0.0003
                                     0.2992 -0.0092  0.0021 -0.7682  0.0213
                                    -0.0037 -0.1992  0.0055 -0.0010 -0.0075
                                    -0.0069  0.0052 -0.0098 -0.0099
              ( 60.87%)  -0.7802* H  74 s( 99.95%)p 0.00(  0.05%)
                                     0.9997  0.0015  0.0005 -0.0081  0.0208
                                     0.0056
1560. (0.02319) BD*( 1) C  45 - C  46
              ( 50.48%)   0.7105* C  45 s( 35.81%)p 1.79( 64.13%)d 0.00(  0.06%)
                                     0.0001  0.5984 -0.0015 -0.0044 -0.0001
                                    -0.2685  0.0021  0.0054  0.7226  0.0119
                                    -0.0097  0.2157  0.0166 -0.0008 -0.0144
                                    -0.0012  0.0096 -0.0151 -0.0088
              ( 49.52%)  -0.7037* C  46 s( 33.92%)p 1.95( 66.03%)d 0.00(  0.05%)
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                                    -0.0001  0.5823  0.0105  0.0032  0.0001
                                     0.2821 -0.0061  0.0072 -0.7397  0.0039
                                    -0.0067 -0.1828 -0.0064  0.0029 -0.0123
                                    -0.0015  0.0091 -0.0133 -0.0076
1561. (0.01777) BD*( 1) C  45 - H  73
              ( 39.23%)   0.6264* C  45 s( 28.08%)p 2.56( 71.89%)d 0.00(  0.04%)
                                     0.0004 -0.5298  0.0108  0.0003 -0.0001
                                    -0.5182  0.0097  0.0075  0.4053 -0.0025
                                    -0.0044 -0.5345  0.0133  0.0097  0.0095
                                    -0.0131  0.0096 -0.0024 -0.0022
              ( 60.77%)  -0.7795* H  73 s( 99.95%)p 0.00(  0.05%)
                                    -0.9997 -0.0022 -0.0013  0.0141 -0.0109
                                     0.0148
1562. (0.03202) BD*( 1) C  46 - C  49
              ( 49.98%)   0.7070* C  46 s( 31.86%)p 2.14( 68.11%)d 0.00(  0.03%)
                                     0.0001 -0.5644  0.0068  0.0036  0.0001
                                    -0.2210 -0.0078  0.0009 -0.3522 -0.0054
                                     0.0021 -0.7127 -0.0147  0.0044 -0.0028
                                    -0.0079 -0.0115  0.0023 -0.0105
              ( 50.02%)  -0.7072* C  49 s( 26.68%)p 2.75( 73.27%)d 0.00(  0.06%)
                                    -0.0001 -0.5165 -0.0013  0.0016  0.0001
                                     0.2369  0.0022 -0.0021  0.3571 -0.0024
                                    -0.0001  0.7410 -0.0012 -0.0030 -0.0047
                                    -0.0095 -0.0147  0.0019 -0.0149
1563. (0.01776) BD*( 1) C  47 - C  48
              ( 49.41%)   0.7029* C  47 s( 25.46%)p 2.93( 74.50%)d 0.00(  0.04%)
                                     0.0001 -0.5044  0.0108 -0.0010  0.0002
                                    -0.4860  0.0006  0.0000 -0.4814 -0.0109
                                    -0.0039  0.5263  0.0032  0.0033 -0.0111
                                     0.0120  0.0111 -0.0025 -0.0007
              ( 50.59%)  -0.7113* C  48 s( 29.04%)p 2.44( 70.91%)d 0.00(  0.04%)
                                    -0.0004 -0.5385  0.0197  0.0031 -0.0001
                                     0.4637  0.0097 -0.0063  0.4668  0.0057
                                    -0.0107 -0.5252 -0.0065  0.0089 -0.0111
                                     0.0124  0.0129  0.0003 -0.0017
1564. (0.01407) BD*( 1) C  47 - C  57
              ( 48.96%)   0.6997* C  47 s( 26.39%)p 2.79( 73.57%)d 0.00(  0.04%)
                                     0.0001 -0.5136  0.0115 -0.0020  0.0004
                                     0.4881  0.0114  0.0033  0.5405 -0.0046
                                     0.0014  0.4528 -0.0053  0.0020 -0.0124
                                    -0.0097 -0.0115  0.0027  0.0006
              ( 51.04%)  -0.7144* C  57 s( 29.01%)p 2.45( 70.94%)d 0.00(  0.05%)
                                    -0.0002 -0.5382  0.0202  0.0029  0.0000
                                    -0.5103 -0.0053  0.0120 -0.4975 -0.0106
                                     0.0068 -0.4483 -0.0050  0.0073 -0.0139
                                    -0.0123 -0.0117 -0.0007  0.0021
1565. (0.02568) BD*( 1) C  47 - H  80
              ( 36.65%)   0.6054* C  47 s( 21.87%)p 3.57( 78.08%)d 0.00(  0.05%)
                                    -0.0001  0.4673  0.0194 -0.0039  0.0000
                                    -0.5302  0.0013  0.0029  0.5421 -0.0107
                                    -0.0021  0.4533 -0.0094 -0.0071 -0.0137
                                    -0.0119  0.0123 -0.0010 -0.0018
              ( 63.35%)  -0.7959* H  80 s( 99.95%)p 0.00(  0.05%)
                                     0.9997 -0.0068  0.0009  0.0164 -0.0118
                                    -0.0100
1566. (0.00771) BD*( 1) C  48 - H 126
              ( 39.06%)   0.6250* C  48 s( 23.30%)p 3.29( 76.66%)d 0.00(  0.04%)
                                    -0.0001  0.4827  0.0059  0.0020  0.0001
                                    -0.5128  0.0049  0.0032  0.4359 -0.0020
                                     0.0064 -0.5599  0.0050 -0.0055 -0.0111
                                     0.0139 -0.0110  0.0012  0.0022
              ( 60.94%)  -0.7807* H 126 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0016  0.0002  0.0143 -0.0089
                                     0.0115
1567. (0.00801) BD*( 1) C  48 - H 127
              ( 39.33%)   0.6272* C  48 s( 24.01%)p 3.16( 75.94%)d 0.00(  0.05%)
                                     0.0000 -0.4899 -0.0038 -0.0015  0.0001
                                    -0.4783  0.0029 -0.0042 -0.5823  0.0008
                                    -0.0058 -0.4376  0.0025  0.0072 -0.0126
                                    -0.0115 -0.0138  0.0024  0.0038
              ( 60.67%)  -0.7789* H 127 s( 99.96%)p 0.00(  0.04%)
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                                    -0.9998 -0.0016  0.0000  0.0094  0.0139
                                     0.0122
1568. (0.01041) BD*( 1) C  48 - H 128
              ( 39.57%)   0.6290* C  48 s( 23.65%)p 3.23( 76.31%)d 0.00(  0.05%)
                                     0.0001 -0.4862 -0.0077  0.0000  0.0000
                                    -0.5408 -0.0011 -0.0065  0.5023 -0.0043
                                    -0.0042  0.4672  0.0000  0.0061  0.0135
                                     0.0111 -0.0119 -0.0021  0.0015
              ( 60.43%)  -0.7774* H 128 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0023 -0.0002  0.0126 -0.0141
                                    -0.0110
1569. (0.01781) BD*( 1) C  49 - C  50
              ( 49.31%)   0.7022* C  49 s( 25.91%)p 2.86( 74.05%)d 0.00(  0.04%)
                                     0.0001 -0.5089  0.0121 -0.0007  0.0000
                                    -0.8477 -0.0045 -0.0039 -0.1466 -0.0136
                                    -0.0017 -0.0129 -0.0021 -0.0017 -0.0045
                                     0.0004 -0.0006 -0.0162  0.0095
              ( 50.69%)  -0.7120* C  50 s( 29.25%)p 2.42( 70.71%)d 0.00(  0.05%)
                                    -0.0003 -0.5405  0.0189  0.0035 -0.0001
                                     0.8273  0.0121 -0.0145  0.1479 -0.0011
                                    -0.0049  0.0197 -0.0025 -0.0008 -0.0068
                                    -0.0005 -0.0002 -0.0170  0.0107
1570. (0.01742) BD*( 1) C  49 - C  58
              ( 48.94%)   0.6996* C  49 s( 26.33%)p 2.80( 73.64%)d 0.00(  0.04%)
                                     0.0001 -0.5130  0.0114 -0.0010 -0.0001
                                     0.2341  0.0099 -0.0001  0.4865 -0.0074
                                     0.0017 -0.6668 -0.0074 -0.0067 -0.0055
                                     0.0063  0.0149  0.0048 -0.0069
              ( 51.06%)  -0.7146* C  58 s( 29.00%)p 2.45( 70.96%)d 0.00(  0.05%)
                                    -0.0003 -0.5383  0.0139 -0.0007  0.0004
                                    -0.2375 -0.0047  0.0061 -0.4655 -0.0082
                                     0.0040  0.6605  0.0035 -0.0083 -0.0059
                                     0.0087  0.0158  0.0042 -0.0090
1571. (0.02452) BD*( 1) C  49 - H  79
              ( 38.53%)   0.6207* C  49 s( 21.13%)p 3.73( 78.82%)d 0.00(  0.05%)
                                     0.0002 -0.4592 -0.0199  0.0003 -0.0001
                                     0.4117 -0.0059 -0.0063 -0.7829  0.0133
                                     0.0022 -0.0741 -0.0010 -0.0059  0.0162
                                     0.0014 -0.0028  0.0113  0.0113
              ( 61.47%)  -0.7840* H  79 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0054 -0.0001 -0.0108  0.0183
                                     0.0007
1572. (0.00762) BD*( 1) C  50 - H 129
              ( 39.26%)   0.6266* C  50 s( 23.28%)p 3.29( 76.68%)d 0.00(  0.04%)
                                     0.0001 -0.4824 -0.0052 -0.0022 -0.0001
                                    -0.2253 -0.0008 -0.0084 -0.4023  0.0020
                                    -0.0031 -0.7444  0.0062 -0.0012 -0.0041
                                    -0.0082 -0.0138  0.0034 -0.0125
              ( 60.74%)  -0.7793* H 129 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0015 -0.0002  0.0034  0.0096
                                     0.0183
1573. (0.01064) BD*( 1) C  50 - H 130
              ( 39.42%)   0.6279* C  50 s( 23.73%)p 3.21( 76.22%)d 0.00(  0.05%)
                                     0.0000 -0.4871 -0.0069 -0.0001  0.0001
                                    -0.4523 -0.0047 -0.0092  0.7450 -0.0039
                                    -0.0006  0.0499  0.0012  0.0002  0.0169
                                     0.0011 -0.0018  0.0089  0.0092
              ( 60.58%)  -0.7783* H 130 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0023 -0.0002  0.0099 -0.0191
                                    -0.0016
1574. (0.00691) BD*( 1) C  50 - H 131
              ( 39.19%)   0.6260* C  50 s( 23.75%)p 3.21( 76.21%)d 0.00(  0.05%)
                                     0.0001 -0.4873 -0.0045 -0.0015  0.0001
                                    -0.2428 -0.0013 -0.0091 -0.5105  0.0030
                                    -0.0027  0.6651 -0.0042 -0.0005 -0.0055
                                     0.0083  0.0156  0.0064 -0.0086
              ( 60.81%)  -0.7798* H 131 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0013 -0.0001  0.0050  0.0122
                                    -0.0157
1575. (0.01736) BD*( 1) C  51 - C  52
              ( 49.30%)   0.7022* C  51 s( 25.89%)p 2.86( 74.08%)d 0.00(  0.04%)
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                                     0.0001 -0.5087  0.0118 -0.0006  0.0000
                                    -0.5288 -0.0133 -0.0036 -0.6263 -0.0001
                                    -0.0006 -0.2621  0.0059 -0.0016 -0.0145
                                    -0.0063 -0.0076  0.0037  0.0071
              ( 50.70%)  -0.7120* C  52 s( 29.26%)p 2.42( 70.70%)d 0.00(  0.04%)
                                    -0.0003 -0.5406  0.0187  0.0032 -0.0001
                                     0.5262  0.0040 -0.0109  0.6035  0.0111
                                    -0.0100  0.2560  0.0041 -0.0035 -0.0166
                                    -0.0066 -0.0077  0.0022  0.0079
1576. (0.01808) BD*( 1) C  51 - C  59
              ( 48.98%)   0.6999* C  51 s( 26.38%)p 2.79( 73.58%)d 0.00(  0.04%)
                                     0.0001 -0.5135  0.0118 -0.0012  0.0000
                                     0.2026 -0.0029 -0.0020  0.5190  0.0130
                                     0.0038 -0.6521  0.0027 -0.0054 -0.0049
                                     0.0062  0.0148  0.0042 -0.0073
              ( 51.02%)  -0.7143* C  59 s( 28.97%)p 2.45( 70.99%)d 0.00(  0.05%)
                                    -0.0003 -0.5379  0.0183  0.0028 -0.0001
                                    -0.1861 -0.0069  0.0027 -0.5215 -0.0055
                                     0.0103  0.6348  0.0075 -0.0083 -0.0053
                                     0.0064  0.0175  0.0064 -0.0071
1577. (0.02484) BD*( 1) C  51 - H  81
              ( 38.55%)   0.6209* C  51 s( 21.11%)p 3.73( 78.83%)d 0.00(  0.05%)
                                     0.0002 -0.4591 -0.0199  0.0002 -0.0001
                                    -0.4307  0.0066 -0.0046  0.4807 -0.0063
                                    -0.0017  0.6095 -0.0112 -0.0073  0.0105
                                     0.0134 -0.0148  0.0009 -0.0047
              ( 61.45%)  -0.7839* H  81 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0053 -0.0003  0.0094 -0.0114
                                    -0.0157
1578. (0.00758) BD*( 1) C  52 - H 114
              ( 39.27%)   0.6266* C  52 s( 23.27%)p 3.30( 76.69%)d 0.00(  0.04%)
                                     0.0001 -0.4824 -0.0049 -0.0019 -0.0002
                                    -0.7336  0.0036 -0.0070  0.3472 -0.0045
                                    -0.0056 -0.3286  0.0026 -0.0021  0.0125
                                    -0.0111  0.0057 -0.0102  0.0053
              ( 60.73%)  -0.7793* H 114 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0015 -0.0002  0.0170 -0.0101
                                     0.0074
1579. (0.00682) BD*( 1) C  52 - H 115
              ( 39.16%)   0.6258* C  52 s( 23.73%)p 3.21( 76.23%)d 0.00(  0.05%)
                                     0.0001 -0.4871 -0.0049 -0.0015  0.0001
                                    -0.2238  0.0001 -0.0067 -0.5221  0.0009
                                    -0.0061  0.6629 -0.0057 -0.0021 -0.0040
                                     0.0078  0.0171  0.0052 -0.0073
              ( 60.84%)  -0.7800* H 115 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0012 -0.0001  0.0049  0.0122
                                    -0.0160
1580. (0.01069) BD*( 1) C  52 - H 116
              ( 39.42%)   0.6279* C  52 s( 23.74%)p 3.21( 76.21%)d 0.00(  0.05%)
                                     0.0000 -0.4872 -0.0066 -0.0001  0.0001
                                     0.3660 -0.0049 -0.0048 -0.4916 -0.0039
                                    -0.0069 -0.6215  0.0014 -0.0034  0.0098
                                     0.0107 -0.0141  0.0030 -0.0062
              ( 60.58%)  -0.7783* H 116 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0023 -0.0002 -0.0102  0.0118
                                     0.0149
1581. (0.01793) BD*( 1) C  53 - C  54
              ( 49.47%)   0.7033* C  53 s( 25.43%)p 2.93( 74.53%)d 0.00(  0.04%)
                                     0.0001 -0.5041  0.0116 -0.0012  0.0002
                                    -0.4120 -0.0070 -0.0017 -0.6126  0.0008
                                    -0.0013  0.4473  0.0101  0.0040 -0.0131
                                     0.0073  0.0118  0.0058  0.0031
              ( 50.53%)  -0.7109* C  54 s( 29.16%)p 2.43( 70.79%)d 0.00(  0.04%)
                                    -0.0004 -0.5397  0.0197  0.0026 -0.0001
                                     0.3913  0.0065 -0.0080  0.5986  0.0106
                                    -0.0085 -0.4428 -0.0038  0.0097 -0.0122
                                     0.0092  0.0136  0.0052  0.0016
1582. (0.01440) BD*( 1) C  53 - C  60
              ( 48.77%)   0.6984* C  53 s( 26.68%)p 2.75( 73.28%)d 0.00(  0.04%)
                                     0.0001 -0.5164  0.0111 -0.0030  0.0003
                                     0.8357 -0.0002  0.0037 -0.0020  0.0130
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                                     0.0010  0.1850  0.0039  0.0027  0.0012
                                    -0.0066  0.0012 -0.0163  0.0085
              ( 51.23%)  -0.7158* C  60 s( 28.89%)p 2.46( 71.06%)d 0.00(  0.05%)
                                    -0.0002 -0.5372  0.0153  0.0008  0.0003
                                    -0.8143 -0.0103  0.0109 -0.0251  0.0000
                                     0.0036 -0.2162  0.0030  0.0031 -0.0017
                                    -0.0094 -0.0008 -0.0178  0.0091
1583. (0.02457) BD*( 1) C  53 - H  82
              ( 37.16%)   0.6096* C  53 s( 21.59%)p 3.63( 78.36%)d 0.00(  0.05%)
                                    -0.0002  0.4642  0.0196 -0.0045 -0.0001
                                     0.3373 -0.0117 -0.0022 -0.7826  0.0088
                                     0.0066 -0.2390  0.0015 -0.0035 -0.0136
                                    -0.0042  0.0084 -0.0116 -0.0090
              ( 62.84%)  -0.7927* H  82 s( 99.95%)p 0.00(  0.05%)
                                     0.9997 -0.0062  0.0008 -0.0052  0.0204
                                     0.0064
1584. (0.00781) BD*( 1) C  54 - H 117
              ( 39.09%)   0.6252* C  54 s( 23.30%)p 3.29( 76.66%)d 0.00(  0.04%)
                                    -0.0002  0.4826  0.0057  0.0020  0.0001
                                    -0.1218  0.0024  0.0046 -0.1206  0.0013
                                     0.0045 -0.8585  0.0068 -0.0062 -0.0001
                                     0.0048  0.0054  0.0005  0.0198
              ( 60.91%)  -0.7804* H 117 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0016  0.0002  0.0044  0.0051
                                     0.0192
1585. (0.01050) BD*( 1) C  54 - H 118
              ( 39.53%)   0.6287* C  54 s( 23.65%)p 3.23( 76.30%)d 0.00(  0.05%)
                                     0.0000 -0.4863 -0.0077  0.0003  0.0000
                                     0.3074 -0.0038 -0.0041 -0.7912 -0.0001
                                    -0.0079 -0.2058  0.0023  0.0041  0.0116
                                     0.0016 -0.0086  0.0127  0.0087
              ( 60.47%)  -0.7777* H 118 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0024 -0.0002 -0.0090  0.0189
                                     0.0062
1586. (0.00765) BD*( 1) C  54 - H 119
              ( 39.46%)   0.6282* C  54 s( 23.89%)p 3.18( 76.06%)d 0.00(  0.05%)
                                     0.0000 -0.4887 -0.0041 -0.0013  0.0001
                                    -0.8584  0.0030 -0.0039  0.0069  0.0003
                                    -0.0068 -0.1538  0.0025  0.0064  0.0010
                                    -0.0071 -0.0021 -0.0185  0.0098
              ( 60.54%)  -0.7781* H 119 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0015  0.0000  0.0201 -0.0025
                                     0.0038
1587. (0.00767) BD*( 1) C  55 - H 108
              ( 39.32%)   0.6271* C  55 s( 23.12%)p 3.32( 76.84%)d 0.00(  0.04%)
                                     0.0002 -0.4808 -0.0082 -0.0040 -0.0002
                                     0.6195 -0.0084  0.0010 -0.5849  0.0036
                                    -0.0137 -0.2050  0.0088 -0.0044  0.0172
                                     0.0052 -0.0061 -0.0019  0.0080
              ( 60.68%)  -0.7790* H 108 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0014 -0.0004 -0.0156  0.0129
                                     0.0053
1588. (0.01032) BD*( 1) C  55 - H 109
              ( 39.46%)   0.6281* C  55 s( 23.70%)p 3.22( 76.26%)d 0.00(  0.04%)
                                     0.0000 -0.4867 -0.0104 -0.0020  0.0001
                                    -0.6609 -0.0017 -0.0052 -0.1029 -0.0056
                                    -0.0091 -0.5612  0.0090 -0.0058 -0.0022
                                    -0.0172 -0.0035 -0.0106 -0.0021
              ( 60.54%)  -0.7781* H 109 s( 99.95%)p 0.00(  0.05%)
                                    -0.9998 -0.0022 -0.0005  0.0161  0.0015
                                     0.0143
1589. (0.00695) BD*( 1) C  55 - H 110
              ( 37.83%)   0.6151* C  55 s( 24.50%)p 3.08( 75.45%)d 0.00(  0.05%)
                                     0.0001 -0.4949  0.0072  0.0057 -0.0004
                                    -0.2873 -0.0032  0.0034 -0.1782 -0.0096
                                    -0.0006  0.7999  0.0022 -0.0116 -0.0025
                                     0.0118  0.0074 -0.0015 -0.0174
              ( 62.17%)  -0.7885* H 110 s( 99.96%)p 0.00(  0.04%)
                                    -0.9998 -0.0013 -0.0005  0.0067  0.0041
                                    -0.0190
1590. (0.00705) BD*( 1) C  56 - H 102
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              ( 39.21%)   0.6262* C  56 s( 23.09%)p 3.33( 76.87%)d 0.00(  0.04%)
                                        -0.0001  0.4804  0.0089 -0.0041  0.0003
                                        -0.1249  0.0045  0.0059 -0.4190  0.0112
                                        -0.0062 -0.7598  0.0050 -0.0113  0.0016
                                         0.0052  0.0150 -0.0034  0.0124
              ( 60.79%)  -0.7796* H 102 s( 99.96%)p 0.00(  0.04%)
                                         0.9998  0.0012  0.0004  0.0046  0.0103
                                         0.0177
1591. (0.00748) BD*( 1) C  56 - H 103
              ( 37.69%)   0.6139* C  56 s( 24.65%)p 3.05( 75.30%)d 0.00(  0.05%)
                                         0.0001 -0.4964  0.0083 -0.0062 -0.0004
                                        -0.1525 -0.0073  0.0016 -0.8364 -0.0016
                                         0.0132  0.1727  0.0074 -0.0005 -0.0066
                                         0.0012  0.0073  0.0176  0.0098
              ( 62.31%)  -0.7894* H 103 s( 99.96%)p 0.00(  0.04%)
                                        -0.9998 -0.0011 -0.0006  0.0026  0.0199
                                        -0.0040
1592. (0.01059) BD*( 1) C  56 - H 104
              ( 39.63%)   0.6295* C  56 s( 23.63%)p 3.23( 76.33%)d 0.00(  0.04%)
                                         0.0000 -0.4860 -0.0113  0.0023  0.0002
                                        -0.7103 -0.0046 -0.0105  0.3397 -0.0091
                                         0.0063 -0.3781  0.0071  0.0016  0.0117
                                        -0.0129  0.0048 -0.0092  0.0039
              ( 60.37%)  -0.7770* H 104 s( 99.95%)p 0.00(  0.05%)
                                        -0.9998 -0.0021 -0.0004  0.0171 -0.0087
                                         0.0098
1593. (0.00670) BD*( 1) C  57 - H 123
              ( 38.50%)   0.6205* C  57 s( 23.50%)p 3.25( 76.46%)d 0.00(  0.04%)
                                        -0.0001  0.4847  0.0041  0.0020  0.0001
                                        -0.5723 -0.0021 -0.0032  0.4761 -0.0065
                                        -0.0046 -0.4584  0.0106 -0.0079 -0.0142
                                         0.0113 -0.0100  0.0025 -0.0011
              ( 61.50%)  -0.7842* H 123 s( 99.96%)p 0.00(  0.04%)
                                         0.9998  0.0012  0.0004  0.0127 -0.0134
                                         0.0083
1594. (0.01162) BD*( 1) C  57 - H 124
              ( 40.02%)   0.6326* C  57 s( 23.56%)p 3.24( 76.39%)d 0.00(  0.04%)
                                         0.0000  0.4854  0.0081  0.0006  0.0002
                                         0.4578 -0.0030 -0.0070 -0.4864 -0.0027
                                        -0.0058 -0.5635 -0.0010 -0.0083 -0.0117
                                        -0.0125  0.0117 -0.0013  0.0034
              ( 59.98%)  -0.7745* H 124 s( 99.95%)p 0.00(  0.05%)
                                         0.9998  0.0023  0.0003 -0.0119  0.0110
                                         0.0138
1595. (0.00660) BD*( 1) C  57 - H 125
              ( 38.70%)   0.6221* C  57 s( 23.93%)p 3.18( 76.03%)d 0.00(  0.05%)
                                        -0.0001  0.4891  0.0053  0.0007 -0.0002
                                        -0.4490 -0.0059 -0.0027 -0.5368  0.0079
                                        -0.0076  0.5200 -0.0042 -0.0040  0.0100
                                        -0.0131 -0.0132 -0.0020  0.0001
              ( 61.30%)  -0.7829* H 125 s( 99.96%)p 0.00(  0.04%)
                                         0.9998  0.0011  0.0002  0.0108  0.0112
                                        -0.0135
1596. (0.00758) BD*( 1) C  58 - H 132
              ( 39.36%)   0.6274* C  58 s( 23.09%)p 3.33( 76.87%)d 0.00(  0.04%)
                                         0.0001 -0.4804 -0.0080 -0.0036 -0.0002
                                        -0.2234  0.0081 -0.0016 -0.3950  0.0048
                                         0.0023 -0.7500  0.0068 -0.0126 -0.0032
                                        -0.0085 -0.0141  0.0025 -0.0120
              ( 60.64%)  -0.7787* H 132 s( 99.96%)p 0.00(  0.04%)
                                        -0.9998 -0.0014 -0.0004  0.0059  0.0111
                                         0.0167
1597. (0.00692) BD*( 1) C  58 - H 133
              ( 38.18%)   0.6179* C  58 s( 24.40%)p 3.10( 75.55%)d 0.00(  0.05%)
                                        -0.0001  0.4939 -0.0070 -0.0052  0.0004
                                        -0.8601 -0.0056  0.0119 -0.1241 -0.0047
                                         0.0003  0.0054  0.0077  0.0028  0.0057
                                        -0.0005  0.0003  0.0187 -0.0115
              ( 61.82%)  -0.7863* H 133 s( 99.96%)p 0.00(  0.04%)
                                         0.9998  0.0014  0.0005  0.0201  0.0021
                                         0.0004
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1598. (0.01074) BD*( 1) C  58 - H 134
              ( 39.69%)   0.6300* C  58 s( 23.52%)p 3.25( 76.43%)d 0.00(  0.04%)
                                        0.0000  0.4849  0.0112  0.0019 -0.0002
                                        0.3910 -0.0078  0.0021 -0.7816  0.0017
                                       -0.0107 -0.0156  0.0035  0.0073 -0.0146
                                        0.0010  0.0014 -0.0108 -0.0106
              ( 60.31%)  -0.7766* H 134 s( 99.95%)p 0.00(  0.05%)
                                        0.9998  0.0022  0.0004 -0.0102  0.0189
                                        0.0016
1599. (0.00771) BD*( 1) C  59 - H 111
              ( 39.41%)   0.6278* C  59 s( 23.12%)p 3.32( 76.83%)d 0.00(  0.04%)
                                        0.0001 -0.4808 -0.0062 -0.0028 -0.0002
                                       -0.7326  0.0062  0.0007  0.3229  0.0010
                                        0.0064 -0.3567  0.0033 -0.0094  0.0117
                                       -0.0122  0.0040 -0.0104  0.0051
              ( 60.59%)  -0.7784* H 111 s( 99.96%)p 0.00(  0.04%)
                                       -0.9998 -0.0015 -0.0003  0.0185 -0.0068
                                        0.0076
1600. (0.01068) BD*( 1) C  59 - H 112
              ( 39.58%)   0.6291* C  59 s( 23.63%)p 3.23( 76.33%)d 0.00(  0.04%)
                                        0.0000 -0.4861 -0.0067 -0.0010  0.0000
                                        0.4396  0.0039  0.0004 -0.4197  0.0069
                                        0.0036 -0.6274 -0.0004 -0.0087  0.0091
                                        0.0121 -0.0129 -0.0015 -0.0056
              ( 60.42%)  -0.7773* H 112 s( 99.95%)p 0.00(  0.05%)
                                       -0.9998 -0.0022 -0.0004 -0.0106  0.0117
                                        0.0148
1601. (0.00685) BD*( 1) C  59 - H 113
              ( 38.27%)   0.6186* C  59 s( 24.28%)p 3.12( 75.68%)d 0.00(  0.05%)
                                       -0.0001  0.4927  0.0030 -0.0004 -0.0002
                                       -0.4846 -0.0001  0.0024 -0.6685  0.0025
                                       -0.0050 -0.2739  0.0040  0.0062  0.0150
                                        0.0067  0.0093 -0.0044 -0.0090
              ( 61.73%)  -0.7857* H 113 s( 99.96%)p 0.00(  0.04%)
                                        0.9998  0.0012 -0.0001  0.0108  0.0140
                                        0.0087
1602. (0.00651) BD*( 1) C  60 - H 120
              ( 38.58%)   0.6211* C  60 s( 23.28%)p 3.29( 76.67%)d 0.00(  0.04%)
                                       -0.0001  0.4824  0.0097  0.0039  0.0000
                                       -0.0866 -0.0017 -0.0098 -0.1992 -0.0066
                                        0.0015 -0.8480  0.0147 -0.0107 -0.0006
                                        0.0031  0.0079 -0.0023  0.0189
              ( 61.42%)  -0.7837* H 120 s( 99.96%)p 0.00(  0.04%)
                                        0.9998  0.0010  0.0004 -0.0003  0.0066
                                        0.0194
1603. (0.00663) BD*( 1) C  60 - H 121
              ( 38.24%)   0.6184* C  60 s( 24.34%)p 3.11( 75.61%)d 0.00(  0.05%)
                                        0.0001 -0.4933  0.0075  0.0046 -0.0002
                                        0.4301  0.0099 -0.0043  0.5960  0.0072
                                       -0.0087 -0.4643  0.0061  0.0081 -0.0134
                                        0.0108  0.0142  0.0045  0.0019
              ( 61.76%)  -0.7859* H 121 s( 99.96%)p 0.00(  0.04%)
                                       -0.9998 -0.0011 -0.0005 -0.0084 -0.0155
                                        0.0093
1604. (0.01163) BD*( 1) C  60 - H 122
              ( 40.17%)   0.6338* C  60 s( 23.50%)p 3.25( 76.46%)d 0.00(  0.04%)
                                        0.0000 -0.4846 -0.0110 -0.0022 -0.0001
                                        0.3784  0.0047  0.0115 -0.7770  0.0058
                                       -0.0074 -0.1321 -0.0001  0.0044  0.0143
                                        0.0025 -0.0044  0.0116  0.0083
              ( 59.83%)  -0.7735* H 122 s( 99.95%)p 0.00(  0.05%)
                                       -0.9998 -0.0022 -0.0004 -0.0079  0.0195
                                        0.0032
1605. (0.00764) BD*( 1) C  61 - H  96
              ( 39.38%)   0.6276* C  61 s( 23.12%)p 3.32( 76.84%)d 0.00(  0.04%)
                                        0.0001 -0.4807 -0.0079 -0.0038 -0.0002
                                        0.0046 -0.0065 -0.0014 -0.2164  0.0009
                                       -0.0106 -0.8493  0.0096 -0.0083  0.0013
                                        0.0001 -0.0080  0.0012 -0.0189
              ( 60.62%)  -0.7786* H  96 s( 99.96%)p 0.00(  0.04%)
                                       -0.9998 -0.0014 -0.0004 -0.0009  0.0037
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                                        0.0205
1606. (0.00685) BD*( 1) C  61 - H  97
              ( 38.03%)   0.6167* C  61 s( 24.44%)p 3.09( 75.51%)d 0.00(  0.05%)
                                       0.0001 -0.4943  0.0071  0.0055 -0.0004
                                      -0.8263 -0.0065  0.0111  0.0357 -0.0087
                                      -0.0030  0.2660 -0.0016 -0.0048  0.0014
                                       0.0112 -0.0003 -0.0177  0.0078
              ( 61.97%)  -0.7872* H  97 s( 99.96%)p 0.00(  0.04%)
                                      -0.9998 -0.0014 -0.0005  0.0195 -0.0012
                                      -0.0061
1607. (0.01033) BD*( 1) C  61 - H  98
              ( 39.51%)   0.6286* C  61 s( 23.60%)p 3.24( 76.36%)d 0.00(  0.04%)
                                       0.0000 -0.4857 -0.0110 -0.0019  0.0002
                                       0.4043 -0.0101  0.0012 -0.6376 -0.0009
                                      -0.0127  0.4397 -0.0012  0.0006  0.0130
                                      -0.0080  0.0128  0.0059  0.0014
              ( 60.49%)  -0.7777* H  98 s( 99.95%)p 0.00(  0.05%)
                                      -0.9998 -0.0021 -0.0003 -0.0107  0.0148
                                      -0.0114
1608. (0.00677) BD*( 1) C  62 - H  87
              ( 39.38%)   0.6276* C  62 s( 22.95%)p 3.36( 77.01%)d 0.00(  0.04%)
                                       0.0001 -0.4790 -0.0048 -0.0031 -0.0001
                                      -0.4665 -0.0025 -0.0026  0.7245 -0.0094
                                       0.0016  0.1651  0.0002  0.0088  0.0160
                                       0.0020 -0.0059  0.0077  0.0091
              ( 60.62%)  -0.7786* H  87 s( 99.96%)p 0.00(  0.04%)
                                      -0.9998 -0.0010 -0.0004  0.0104 -0.0174
                                      -0.0020
1609. (0.01126) BD*( 1) C  62 - H  88
              ( 39.97%)   0.6322* C  62 s( 23.44%)p 3.26( 76.52%)d 0.00(  0.05%)
                                       0.0000 -0.4841 -0.0073 -0.0009 -0.0001
                                       0.6110 -0.0038 -0.0039 -0.0685 -0.0033
                                       0.0011  0.6221  0.0039  0.0118  0.0025
                                      -0.0190  0.0006 -0.0079 -0.0045
              ( 60.03%)  -0.7748* H  88 s( 99.96%)p 0.00(  0.04%)
                                      -0.9998 -0.0022 -0.0003 -0.0154  0.0015
                                      -0.0145
1610. (0.00967) BD*( 1) C  62 - H  89
              ( 36.82%)   0.6068* C  62 s( 25.12%)p 2.98( 74.84%)d 0.00(  0.05%)
                                       0.0001 -0.5011 -0.0065  0.0008  0.0002
                                      -0.5279 -0.0010 -0.0013 -0.6832  0.0088
                                      -0.0011  0.0533 -0.0011  0.0090 -0.0174
                                      -0.0007  0.0019  0.0040  0.0120
              ( 63.18%)  -0.7948* H  89 s( 99.95%)p 0.00(  0.05%)
                                      -0.9997 -0.0022  0.0000  0.0130  0.0184
                                       0.0042
```

NHO Directionality and "Bond Bending" (deviations from line of nuclear centers)

[Thresholds for printing: angular deviation > 1.0 degree]
hybrid p-character > 25.0%
orbital occupancy > 0.10e

NBO	Line of Centers		Hybrid 1			Hybrid 2		
	Theta	Phi	Theta	Phi	Dev	Theta	Phi	Dev
1. BD (1) C 1 - O 2	161.8	128.3	160.9	122.8	2.0	17.4	316.1	2.5
2. BD (2) C 1 - O 2	161.8	128.3	108.0	286.0	88.9	105.8	284.2	89.2
3. BD (1) C 1 - B 14	46.2	4.9	71.1	10.8	25.4	153.5	176.6	20.2
4. BD (1) C 1 - B 15	24.7	247.1	50.6	211.4	33.0	159.6	128.4	22.8
5. BD (1) C 3 - C 4	63.0	330.8	64.0	330.1	1.2	--	--	--
6. BD (1) C 3 - C 8	56.4	133.5	57.6	133.9	1.2	125.8	312.7	2.4
7. BD (2) C 3 - C 8	56.4	133.5	77.0	233.3	90.8	104.1	53.2	90.0
8. BD (1) C 3 - C 53	167.9	215.3	166.7	216.9	1.2	10.9	38.0	1.3
9. BD (1) C 4 - C 5	16.8	36.9	--	--	--	163.4	221.3	1.3
10. BD (2) C 4 - C 5	16.8	36.9	75.1	234.4	91.2	73.2	235.0	90.8
11. BD (1) C 4 - N 9	122.0	315.1	--	--	--	59.9	135.9	2.0
12. BD (1) C 5 - C 6	58.7	134.7	57.6	133.9	1.2	118.9	315.7	2.5
13. BD (1) C 5 - C 51	64.3	334.6	64.5	333.3	1.2	--	--	--

14.	BD (| 1)	C	6	- C	7	115.5	151.6	110.8	150.7	4.7	59.9	332.6	4.7
15.	BD (| 2)	C	6	- C	7	115.5	151.6	105.4	54.6	89.5	104.9	53.9	89.7
17.	BD (| 1)	C	7	- C	8	164.9	219.8	163.0	204.9	4.5	14.3	57.0	4.4
20.	BD (| 1)	N	9	- C	10	96.6	263.2	96.3	259.4	3.8	81.9	87.8	4.8
21.	BD (| 2)	N	9	- C	10	96.6	263.2	149.3	156.8	92.6	27.0	339.4	90.3
22.	BD (| 1)	N	9	- C	13	112.1	18.8	110.9	22.1	3.2	66.7	192.0	6.4
23.	BD (| 1)	C	10	- N	11	117.3	341.4	118.4	335.3	5.5	63.9	165.8	4.1
24.	BD (| 1)	C	10	- B	14	82.6	211.6	75.4	215.3	8.0	90.0	27.9	8.3
25.	BD (| 1)	N	11	- C	12	98.8	52.6	99.3	49.4	3.2	83.8	238.4	6.3
26.	BD (| 1)	N	11	- C	41	102.0	287.1	103.4	285.3	2.3	79.3	109.1	2.4
27.	BD (| 2)	N	11	- C	41	102.0	287.1	154.5	162.9	92.8	14.9	352.2	84.5
28.	BD (| 1)	C	12	- C	13	68.8	119.8	72.1	109.9	9.9	114.1	310.0	9.9
29.	BD (| 2)	C	12	- C	13	68.8	119.8	152.7	161.1	90.0	152.7	160.8	90.0
30.	BD (| 1)	C	12	- H	71	116.6	353.3	116.6	354.9	1.4	--	--	--
31.	BD (| 1)	C	13	- H	72	88.4	73.7	89.1	72.6	1.3	--	--	--
32.	BD (| 1)	B	14	- B	15	81.2	205.6	46.3	226.0	39.1	67.8	13.8	33.1
33.	BD (| 1)	B	15	- C	16	63.9	215.9	60.0	215.7	3.9	112.6	36.8	3.6
34.	BD (| 1)	C	16	- N	17	107.2	182.2	111.5	179.6	4.9	76.4	3.4	3.8
35.	BD (| 2)	C	16	- N	17	107.2	182.2	49.5	107.9	89.7	133.0	286.0	92.1
36.	BD (| 1)	C	16	- N	20	42.0	273.8	41.6	282.0	5.5	137.9	88.7	3.4
37.	BD (| 1)	N	17	- C	18	57.1	232.0	58.7	228.5	3.3	126.5	58.5	6.5
38.	BD (| 1)	N	17	- C	21	133.3	126.1	134.7	125.7	1.4	47.1	307.7	1.3
39.	BD (| 1)	C	18	- C	19	48.9	327.4	45.1	314.5	10.2	126.0	158.8	10.2
40.	BD (| 2)	C	18	- C	19	48.9	327.4	131.8	287.7	90.3	131.5	288.3	90.2
41.	BD (| 1)	C	18	- H	63	99.0	189.3	98.0	190.4	1.5	--	--	--
42.	BD (| 1)	C	19	- N	20	98.6	25.8	93.8	21.2	6.6	79.0	208.0	3.3
43.	BD (| 1)	C	19	- H	64	45.5	259.2	46.1	257.3	1.5	--	--	--
44.	BD (| 1)	N	20	- C	31	54.3	346.8	56.2	345.7	2.1	126.5	166.0	1.0
45.	BD (| 1)	C	21	- C	22	163.2	270.9	162.1	271.3	1.1	15.4	89.6	1.4
46.	BD (| 1)	C	21	- C	26	71.6	119.4	70.5	119.6	1.2	106.8	299.2	1.6
47.	BD (| 2)	C	21	- C	26	71.6	119.4	97.5	30.6	91.2	98.0	32.4	90.3
48.	BD (| 1)	C	22	- C	23	130.9	129.4	132.2	130.0	1.4	51.3	308.8	2.3
49.	BD (| 2)	C	22	- C	23	130.9	129.4	98.3	30.7	91.1	98.4	31.9	89.9
51.	BD (| 1)	C	23	- C	24	73.0	119.3	77.4	120.0	4.4	111.4	298.5	4.5
53.	BD (| 1)	C	24	- C	25	15.5	89.1	19.5	97.3	4.6	167.9	256.1	4.6
54.	BD (| 2)	C	24	- C	25	15.5	89.1	98.4	31.8	89.9	81.3	211.8	90.2
56.	BD (| 1)	C	25	- C	26	46.6	310.1	44.2	310.8	2.4	132.1	129.8	1.3
59.	BD (| 1)	C	27	- C	28	88.0	229.5	87.2	230.2	1.0	--	--	--
71.	BD (| 1)	C	31	- C	32	29.4	82.3	--	--	--	150.9	259.7	1.3
72.	BD (| 1)	C	31	- C	36	106.5	313.2	--	--	--	74.8	133.6	1.3
73.	BD (| 2)	C	31	- C	36	106.5	313.2	117.3	53.8	91.5	117.8	51.0	91.0
74.	BD (| 1)	C	32	- C	33	53.9	344.5	52.8	345.2	1.3	124.0	162.8	2.5
75.	BD (| 2)	C	32	- C	33	53.9	344.5	116.0	53.7	90.1	116.8	53.0	89.9
77.	BD (| 1)	C	33	- C	34	105.5	314.3	101.7	316.9	4.5	70.6	131.8	4.5
79.	BD (| 1)	C	34	- C	35	150.2	258.8	148.1	266.5	4.5	28.2	70.2	4.5
80.	BD (| 2)	C	34	- C	35	150.2	258.8	62.9	232.3	89.9	62.8	231.9	89.9
82.	BD (| 1)	C	35	- C	36	128.4	165.6	130.4	167.3	2.4	52.7	344.8	1.3
97.	BD (| 1)	C	41	- C	42	150.7	237.0	135.8	243.9	15.5	29.8	59.2	1.2
98.	BD (| 1)	C	41	- C	46	49.7	322.6	71.6	318.2	22.2	129.2	141.7	1.2
99.	BD (| 2)	C	41	- C	46	49.7	322.6	110.4	25.0	83.8	63.1	207.9	90.5
100.	BD (| 1)	C	42	- C	43	102.1	291.6	102.8	290.5	1.3	79.8	113.2	2.4
101.	BD (| 2)	C	42	- C	43	102.1	291.6	64.4	206.6	90.8	116.0	28.1	89.6
103.	BD (| 1)	C	43	- C	44	50.7	322.0	54.2	318.6	4.4	132.9	145.7	4.6
105.	BD (| 1)	C	44	- C	45	29.9	59.0	28.1	50.0	4.7	147.7	246.9	4.7
106.	BD (| 2)	C	44	- C	45	29.9	59.0	116.4	28.2	90.1	116.3	28.3	90.0
108.	BD (| 1)	C	45	- C	46	75.6	110.7	73.3	109.8	2.5	103.2	290.9	1.2
112.	BD (| 1)	C	47	- C	57	121.9	225.8	121.4	226.9	1.0	--	--	--
158.	BD (| 1)	C	62	- H	89	92.6	52.5	94.1	51.9	1.6	--	--	--
221.	LP (| 1)	O	2			--	--	163.2	113.8	--	--	--	--
222.	LP (| 2)	O	2			--	--	83.9	196.1	--	--	--	--
223.	LP*(| 1)	B	14			--	--	74.6	119.0	--	--	--	--
224.	LP (| 1)	B	15			--	--	69.5	112.8	--	--	--	--
225.	LP (| 1)	N	20			--	--	130.1	289.5	--	--	--	--
1454.	BD*(| 2)	C	1	- O	2	161.8	128.3	108.0	286.0	88.9	105.8	284.2	89.2
1455.	BD*(| 1)	C	1	- B	14	46.2	4.9	71.1	10.8	25.4	153.5	176.6	20.2
1459.	BD*(| 2)	C	3	- C	8	56.4	133.5	77.0	233.3	90.8	104.1	53.2	90.0
1462.	BD*(| 2)	C	4	- C	5	16.8	36.9	75.1	234.4	91.2	73.2	235.0	90.8
1467.	BD*(| 2)	C	6	- C	7	115.5	151.6	105.4	54.6	89.5	104.9	53.9	89.7
1473.	BD*(| 2)	N	9	- C	10	96.6	263.2	149.3	156.8	92.6	27.0	339.4	90.3
1479.	BD*(| 2)	N	11	- C	41	102.0	287.1	154.5	162.9	92.8	14.9	352.2	84.5
1481.	BD*(| 2)	C	12	- C	13	68.8	119.8	152.7	161.1	90.0	152.7	160.8	90.0

1487. BD*(2) C 16 - N 17	107.2	182.2	49.5	107.9	89.7	133.0	286.0	92.1
1492. BD*(2) C 18 - C 19	48.9	327.4	131.8	287.7	90.3	131.5	288.3	90.2
1499. BD*(2) C 21 - C 26	71.6	119.4	97.5	30.6	91.2	98.0	32.4	90.3
1501. BD*(2) C 22 - C 23	130.9	129.4	98.3	30.7	91.1	98.4	31.9	89.9
1506. BD*(2) C 24 - C 25	15.5	89.1	98.4	31.8	89.9	81.3	211.8	90.2
1525. BD*(2) C 31 - C 36	106.5	313.2	117.3	53.8	91.5	117.8	51.0	91.0
1527. BD*(2) C 32 - C 33	53.9	344.5	116.0	53.7	90.1	116.8	53.0	89.9
1532. BD*(2) C 34 - C 35	150.2	258.8	62.9	232.3	89.9	62.8	231.9	89.9
1551. BD*(2) C 41 - C 46	49.7	322.6	110.4	25.0	83.8	63.1	207.9	90.5
1553. BD*(2) C 42 - C 43	102.1	291.6	64.4	206.6	90.8	116.0	28.1	89.6
1558. BD*(2) C 44 - C 45	29.9	59.0	116.4	28.2	90.1	116.3	28.3	90.0

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - O 2	/226. RY*(1) C 1	1.44	1.92	0.047
1. BD (1) C 1 - O 2	/422. RY*(1) B 15	0.51	2.53	0.032
1. BD (1) C 1 - O 2	/***. BD*(1) C 1 - B 14	1.51	1.24	0.040
1. BD (1) C 1 - O 2	/***. BD*(1) C 1 - B 15	2.00	1.35	0.047
2. BD (2) C 1 - O 2	/223. LP*(1) B 14	2.48	0.29	0.028
2. BD (2) C 1 - O 2	/224. LP (1) B 15	3.43	0.29	0.035
2. BD (2) C 1 - O 2	/***. BD*(2) C 1 - O 2	0.94	0.30	0.017
3. BD (1) C 1 - B 14	/224. LP (1) B 15	0.67	0.35	0.015
3. BD (1) C 1 - B 14	/229. RY*(4) C 1	0.56	2.08	0.033
3. BD (1) C 1 - B 14	/240. RY*(1) O 2	1.23	1.18	0.037
3. BD (1) C 1 - B 14	/242. RY*(3) O 2	0.77	1.58	0.034
3. BD (1) C 1 - B 14	/***. BD*(1) C 1 - B 14	1.69	0.65	0.031
3. BD (1) C 1 - B 14	/***. BD*(1) C 1 - B 15	10.68	0.77	0.086
3. BD (1) C 1 - B 14	/***. BD*(1) N 9 - C 10	0.64	0.67	0.020
3. BD (1) C 1 - B 14	/***. BD*(2) N 9 - C 10	11.08	0.27	0.055
3. BD (1) C 1 - B 14	/***. BD*(1) B 14 - B 15	10.07	0.80	0.086
3. BD (1) C 1 - B 14	/***. BD*(1) B 15 - C 16	28.64	0.73	0.138
4. BD (1) C 1 - B 15	/223. LP*(1) B 14	1.99	0.43	0.030
4. BD (1) C 1 - B 15	/240. RY*(1) O 2	1.35	1.26	0.038
4. BD (1) C 1 - B 15	/242. RY*(3) O 2	1.28	1.66	0.043
4. BD (1) C 1 - B 15	/413. RY*(6) B 14	0.78	3.86	0.051
4. BD (1) C 1 - B 15	/430. RY*(9) B 15	1.15	6.86	0.082
4. BD (1) C 1 - B 15	/433. RY*(12) B 15	0.71	4.38	0.051

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   4. BD (   1) C   1 - B  15        /436. RY*(   1) C  16                  1.14    2.22
0.046
   4. BD (   1) C   1 - B  15        /***. BD*(   1) C   1 - O   2          2.08    0.92
0.040
   4. BD (   1) C   1 - B  15        /***. BD*(   1) C   1 - B  14          4.92    0.74
0.054
   4. BD (   1) C   1 - B  15        /***. BD*(   1) C   1 - B  15          0.87    0.85
0.025
   4. BD (   1) C   1 - B  15        /***. BD*(   1) C  10 - B  14         12.72    0.84
0.095
   4. BD (   1) C   1 - B  15        /***. BD*(   1) B  14 - B  15          3.90    0.89
0.054
   4. BD (   1) C   1 - B  15        /***. BD*(   1) B  15 - C  16          2.57    0.81
0.042
   4. BD (   1) C   1 - B  15        /***. BD*(   2) C  16 - N  17          0.65    0.34
0.015
   4. BD (   1) C   1 - B  15        /***. BD*(   1) C  16 - N  20          4.04    0.76
0.050
   5. BD (   1) C   3 - C   4        /283. RY*(   2) C   5                  0.63    1.59
0.028
   5. BD (   1) C   3 - C   4        /338. RY*(   1) N   9                  0.68    1.49
0.029
   5. BD (   1) C   3 - C   4        /***. BD*(   1) C   3 - C   8          1.26    1.10
0.033
   5. BD (   1) C   3 - C   4        /***. BD*(   1) C   3 - C  53          0.58    0.96
0.021
   5. BD (   1) C   3 - C   4        /***. BD*(   1) C   4 - C   5          2.31    1.09
0.045
   5. BD (   1) C   3 - C   4        /***. BD*(   1) C   5 - C  51          3.72    0.95
0.053
   5. BD (   1) C   3 - C   4        /***. BD*(   1) C   8 - H  76          2.91    0.98
0.048
   5. BD (   1) C   3 - C   4        /***. BD*(   1) N   9 - C  10          1.28    0.98
0.032
   5. BD (   1) C   3 - C   4        /***. BD*(   1) N   9 - C  13          1.29    0.97
0.032
   5. BD (   1) C   3 - C   4        /***. BD*(   1) C  53 - C  60          1.15    0.94
0.029
   6. BD (   1) C   3 - C   8        /268. RY*(   1) C   4                  0.88    1.98
0.038
   6. BD (   1) C   3 - C   8        /311. RY*(   2) C   7                  0.93    1.83
0.037
   6. BD (   1) C   3 - C   8        /953. RY*(   1) C  53                  0.58    1.68
0.028
   6. BD (   1) C   3 - C   8        /***. BD*(   1) C   3 - C   4          1.47    1.09
0.036
   6. BD (   1) C   3 - C   8        /***. BD*(   1) C   3 - C  53          0.71    0.96
0.023
   6. BD (   1) C   3 - C   8        /***. BD*(   1) C   4 - N   9          5.06    0.94
0.062
   6. BD (   1) C   3 - C   8        /***. BD*(   1) C   7 - C   8          1.57    1.11
0.037
   6. BD (   1) C   3 - C   8        /***. BD*(   1) C   7 - H  77          2.54    0.97
0.044
   6. BD (   1) C   3 - C   8        /***. BD*(   1) C  53 - H  82          0.84    0.98
0.026
   7. BD (   2) C   3 - C   8        /312. RY*(   3) C   7                  1.05    0.76
0.028
   7. BD (   2) C   3 - C   8        /***. BD*(   2) C   4 - C   5         14.14    0.23
0.051
   7. BD (   2) C   3 - C   8        /***. BD*(   2) C   6 - C   7         16.54    0.22
0.054
   7. BD (   2) C   3 - C   8        /***. BD*(   1) C  53 - C  54          2.53    0.51
0.035
   7. BD (   2) C   3 - C   8        /***. BD*(   1) C  53 - C  60          0.69    0.53
0.019
   7. BD (   2) C   3 - C   8        /***. BD*(   1) C  53 - H  82          0.65    0.57
0.019
   8. BD (   1) C   3 - C  53        /268. RY*(   1) C   4                  1.49    1.90
0.048
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   8. BD (   1) C   3 - C  53        /324. RY*(   1) C   8                0.89    1.95
0.037
   8. BD (   1) C   3 - C  53        /***. BD*(   1) C   3 - C   4        0.71    1.00
0.024
   8. BD (   1) C   3 - C  53        /***. BD*(   1) C   3 - C   8        0.78    1.02
0.025
   8. BD (   1) C   3 - C  53        /***. BD*(   1) C   4 - C   5        3.90    1.00
0.056
   8. BD (   1) C   3 - C  53        /***. BD*(   1) C   7 - C   8        2.82    1.03
0.048
   8. BD (   1) C   3 - C  53        /***. BD*(   1) C  54 - H 117        1.48    0.88
0.032
   8. BD (   1) C   3 - C  53        /***. BD*(   1) C  60 - H 120        1.15    0.89
0.029
   9. BD (   1) C   4 - C   5        /255. RY*(   2) C   3                0.86    1.72
0.035
   9. BD (   1) C   4 - C   5        /297. RY*(   2) C   6                0.52    1.74
0.027
   9. BD (   1) C   4 - C   5        /338. RY*(   1) N   9                0.80    1.49
0.031
   9. BD (   1) C   4 - C   5        /***. BD*(   1) C   3 - C   4        2.31    1.09
0.045
   9. BD (   1) C   4 - C   5        /***. BD*(   1) C   3 - C  53        3.52    0.97
0.052
   9. BD (   1) C   4 - C   5        /***. BD*(   1) C   4 - N   9        0.50    0.94
0.019
   9. BD (   1) C   4 - C   5        /***. BD*(   1) C   5 - C   6        1.40    1.10
0.035
   9. BD (   1) C   4 - C   5        /***. BD*(   1) C   5 - C  51        0.60    0.95
0.021
   9. BD (   1) C   4 - C   5        /***. BD*(   1) C   6 - H  78        2.88    0.98
0.047
   9. BD (   1) C   4 - C   5        /***. BD*(   1) N   9 - C  10        1.48    0.98
0.034
   9. BD (   1) C   4 - C   5        /***. BD*(   2) N   9 - C  10        0.76    0.59
0.023
   9. BD (   1) C   4 - C   5        /***. BD*(   1) N   9 - C  13        0.72    0.97
0.024
   9. BD (   1) C   4 - C   5        /***. BD*(   1) C  51 - C  52        0.59    0.91
0.021
   9. BD (   1) C   4 - C   5        /***. BD*(   1) C  51 - C  59        0.65    0.92
0.022
  10. BD (   2) C   4 - C   5        /298. RY*(   3) C   6                1.47    0.77
0.033
  10. BD (   2) C   4 - C   5        /***. BD*(   2) C   3 - C   8       16.45    0.24
0.056
  10. BD (   2) C   4 - C   5        /***. BD*(   2) C   6 - C   7       13.56    0.23
0.050
  10. BD (   2) C   4 - C   5        /***. BD*(   1) N   9 - C  10        3.25    0.57
0.042
  10. BD (   2) C   4 - C   5        /***. BD*(   1) N   9 - C  13        3.02    0.57
0.040
  10. BD (   2) C   4 - C   5        /***. BD*(   1) C  51 - C  52        2.10    0.51
0.032
  10. BD (   2) C   4 - C   5        /***. BD*(   1) C  51 - C  59        2.33    0.51
0.034
  11. BD (   1) C   4 - N   9        /254. RY*(   1) C   3                0.71    2.07
0.034
  11. BD (   1) C   4 - N   9        /282. RY*(   1) C   5                0.58    2.11
0.031
  11. BD (   1) C   4 - N   9        /352. RY*(   1) C  10                0.82    2.35
0.039
  11. BD (   1) C   4 - N   9        /395. RY*(   2) C  13                0.68    2.04
0.033
  11. BD (   1) C   4 - N   9        /***. BD*(   1) C   3 - C   4        0.61    1.17
0.024
  11. BD (   1) C   4 - N   9        /***. BD*(   1) C   3 - C   8        2.37    1.19
0.047
  11. BD (   1) C   4 - N   9        /***. BD*(   1) C   4 - C   5        0.51    1.17
0.022
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  11. BD (   1) C   4 - N   9        /***. BD*(   1) C   5 - C   6           2.28    1.18
0.046
  11. BD (   1) C   4 - N   9        /***. BD*(   1) N   9 - C  10           0.84    1.06
0.027
  11. BD (   1) C   4 - N   9        /***. BD*(   1) N   9 - C  13           0.56    1.05
0.022
  11. BD (   1) C   4 - N   9        /***. BD*(   1) C  10 - N  11           1.32    1.06
0.034
  11. BD (   1) C   4 - N   9        /***. BD*(   1) C  12 - C  13           0.87    1.21
0.029
  12. BD (   1) C   5 - C   6        /268. RY*(   1) C   4                  0.87    1.99
0.037
  12. BD (   1) C   5 - C   6        /311. RY*(   2) C   7                  0.96    1.84
0.038
  12. BD (   1) C   5 - C   6        /925. RY*(   1) C  51                  0.74    1.75
0.032
  12. BD (   1) C   5 - C   6        /***. BD*(   1) C   4 - C   5          1.57    1.09
0.037
  12. BD (   1) C   5 - C   6        /***. BD*(   1) C   4 - N   9          4.93    0.94
0.061
  12. BD (   1) C   5 - C   6        /***. BD*(   1) C   5 - C  51          0.68    0.95
0.023
  12. BD (   1) C   5 - C   6        /***. BD*(   1) C   6 - C   7          1.58    1.12
0.038
  12. BD (   1) C   5 - C   6        /***. BD*(   1) C   7 - H  77          2.56    0.97
0.045
  12. BD (   1) C   5 - C   6        /***. BD*(   1) C  51 - H  81          1.05    0.95
0.028
  13. BD (   1) C   5 - C  51        /268. RY*(   1) C   4                  1.49    1.91
0.048
  13. BD (   1) C   5 - C  51        /296. RY*(   1) C   6                  0.92    1.98
0.038
  13. BD (   1) C   5 - C  51        /***. BD*(   1) C   3 - C   4          3.73    1.01
0.055
  13. BD (   1) C   5 - C  51        /***. BD*(   1) C   4 - C   5          0.73    1.01
0.024
  13. BD (   1) C   5 - C  51        /***. BD*(   1) C   5 - C   6          0.73    1.02
0.024
  13. BD (   1) C   5 - C  51        /***. BD*(   1) C   6 - C   7          2.75    1.04
0.048
  13. BD (   1) C   5 - C  51        /***. BD*(   1) C  52 - H 114          1.41    0.87
0.031
  13. BD (   1) C   5 - C  51        /***. BD*(   1) C  59 - H 111          1.40    0.87
0.031
  14. BD (   1) C   6 - C   7        /282. RY*(   1) C   5                  1.36    2.04
0.047
  14. BD (   1) C   6 - C   7        /324. RY*(   1) C   8                  0.52    2.05
0.029
  14. BD (   1) C   6 - C   7        /325. RY*(   2) C   8                  0.58    1.62
0.027
  14. BD (   1) C   6 - C   7        /***. BD*(   1) C   5 - C   6          1.81    1.11
0.040
  14. BD (   1) C   6 - C   7        /***. BD*(   1) C   5 - C  51          4.01    0.96
0.056
  14. BD (   1) C   6 - C   7        /***. BD*(   1) C   7 - C   8          1.49    1.12
0.037
  14. BD (   1) C   6 - C   7        /***. BD*(   1) C   8 - H  76          2.55    0.99
0.045
  15. BD (   2) C   6 - C   7        /***. BD*(   2) C   3 - C   8         13.21    0.24
0.050
  15. BD (   2) C   6 - C   7        /***. BD*(   2) C   4 - C   5         16.26    0.23
0.055
  16. BD (   1) C   6 - H  78        /282. RY*(   1) C   5                  1.68    1.86
0.050
  16. BD (   1) C   6 - H  78        /310. RY*(   1) C   7                  1.01    1.66
0.037
  16. BD (   1) C   6 - H  78        /***. BD*(   1) C   4 - C   5          5.20    0.91
0.062
  16. BD (   1) C   6 - H  78        /***. BD*(   1) C   7 - C   8          3.89    0.94
0.054
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  17. BD (   1) C   7 - C   8        /254. RY*(   1) C   3                1.30    1.99
0.046
  17. BD (   1) C   7 - C   8        /297. RY*(   2) C   6                0.67    1.74
0.031
  17. BD (   1) C   7 - C   8        /***. BD*(   1) C   3 - C   8        1.78    1.11
0.040
  17. BD (   1) C   7 - C   8        /***. BD*(   1) C   3 - C  53        4.02    0.97
0.056
  17. BD (   1) C   7 - C   8        /***. BD*(   1) C   6 - C   7        1.51    1.12
0.037
  17. BD (   1) C   7 - C   8        /***. BD*(   1) C   6 - H  78        2.68    0.98
0.046
  18. BD (   1) C   7 - H  77        /296. RY*(   1) C   6                1.42    1.88
0.046
  18. BD (   1) C   7 - H  77        /324. RY*(   1) C   8                1.44    1.87
0.046
  18. BD (   1) C   7 - H  77        /***. RY*(   1) H  78                0.51    1.07
0.021
  18. BD (   1) C   7 - H  77        /***. BD*(   1) C   3 - C   8        4.55    0.93
0.058
  18. BD (   1) C   7 - H  77        /***. BD*(   1) C   5 - C   6        4.50    0.93
0.058
  19. BD (   1) C   8 - H  76        /254. RY*(   1) C   3                1.64    1.81
0.049
  19. BD (   1) C   8 - H  76        /310. RY*(   1) C   7                1.00    1.66
0.036
  19. BD (   1) C   8 - H  76        /***. BD*(   1) C   3 - C   4        5.19    0.91
0.061
  19. BD (   1) C   8 - H  76        /***. BD*(   1) C   6 - C   7        3.97    0.94
0.055
  20. BD (   1) N   9 - C  10        /223. LP*(   1) B  14                0.70    0.75
0.024
  20. BD (   1) N   9 - C  10        /269. RY*(   2) C   4                0.90    1.47
0.033
  20. BD (   1) N   9 - C  10        /396. RY*(   3) C  13                0.66    1.78
0.031
  20. BD (   1) N   9 - C  10        /***. BD*(   1) C   3 - C   4        0.56    1.18
0.023
  20. BD (   1) N   9 - C  10        /***. BD*(   1) C   4 - C   5        0.72    1.18
0.026
  20. BD (   1) N   9 - C  10        /***. BD*(   2) C   4 - C   5        0.96    0.73
0.026
  20. BD (   1) N   9 - C  10        /***. BD*(   1) C   4 - N   9        0.94    1.03
0.028
  20. BD (   1) N   9 - C  10        /***. BD*(   1) N   9 - C  13        0.90    1.06
0.028
  20. BD (   1) N   9 - C  10        /***. BD*(   1) C  10 - B  14        1.74    1.16
0.040
  20. BD (   1) N   9 - C  10        /***. BD*(   1) N  11 - C  41        4.89    1.03
0.063
  20. BD (   1) N   9 - C  10        /***. BD*(   1) C  13 - H  72        2.42    1.06
0.045
  20. BD (   1) N   9 - C  10        /***. BD*(   1) B  14 - B  15        1.01    1.20
0.031
  21. BD (   2) N   9 - C  10        /270. RY*(   3) C   4                1.02    1.43
0.035
  21. BD (   2) N   9 - C  10        /394. RY*(   1) C  13                2.14    0.95
0.042
  21. BD (   2) N   9 - C  10        /***. BD*(   1) C   1 - B  14        1.43    0.62
0.027
  21. BD (   2) N   9 - C  10        /***. BD*(   1) C   3 - C   4        4.06    0.75
0.050
  21. BD (   2) N   9 - C  10        /***. BD*(   1) C   4 - C   5        4.08    0.75
0.051
  21. BD (   2) N   9 - C  10        /***. BD*(   2) C  12 - C  13       15.90    0.27
0.061
  21. BD (   2) N   9 - C  10        /***. BD*(   1) B  14 - B  15        0.53    0.77
0.018
  22. BD (   1) N   9 - C  13        /269. RY*(   2) C   4                0.69    1.47
0.029
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  22. BD (   1) N   9 - C  13        /352. RY*(   1) C  10                  0.64    2.36
0.035
  22. BD (   1) N   9 - C  13        /354. RY*(   3) C  10                  0.66    2.40
0.036
  22. BD (   1) N   9 - C  13        /355. RY*(   4) C  10                  0.51    2.31
0.031
  22. BD (   1) N   9 - C  13        /382. RY*(   3) C  12                  0.87    1.79
0.035
  22. BD (   1) N   9 - C  13        /***. BD*(   1) C   3 - C   4          0.95    1.18
0.030
  22. BD (   1) N   9 - C  13        /***. BD*(   2) C   4 - C   5          1.18    0.73
0.029
  22. BD (   1) N   9 - C  13        /***. BD*(   1) C   4 - N   9          0.82    1.03
0.026
  22. BD (   1) N   9 - C  13        /***. BD*(   1) N   9 - C  10          0.84    1.07
0.027
  22. BD (   1) N   9 - C  13        /***. BD*(   1) C  10 - N  11          0.63    1.07
0.023
  22. BD (   1) N   9 - C  13        /***. BD*(   1) C  10 - B  14          2.77    1.16
0.051
  22. BD (   1) N   9 - C  13        /***. BD*(   1) N  11 - C  41          0.67    1.03
0.024
  22. BD (   1) N   9 - C  13        /***. BD*(   1) C  12 - C  13          0.67    1.22
0.026
  22. BD (   1) N   9 - C  13        /***. BD*(   1) C  12 - H  71          3.70    1.06
0.056
  23. BD (   1) C  10 - N  11        /382. RY*(   3) C  12                  0.63    1.79
0.030
  23. BD (   1) C  10 - N  11        /787. RY*(   2) C  41                  0.83    1.51
0.032
  23. BD (   1) C  10 - N  11        /***. BD*(   1) C   4 - N   9          4.72    1.03
0.062
  23. BD (   1) C  10 - N  11        /***. BD*(   1) C  10 - B  14          1.75    1.16
0.040
  23. BD (   1) C  10 - N  11        /***. BD*(   1) N  11 - C  12          0.92    1.06
0.028
  23. BD (   1) C  10 - N  11        /***. BD*(   1) N  11 - C  41          0.94    1.03
0.028
  23. BD (   1) C  10 - N  11        /***. BD*(   1) C  12 - H  71          2.37    1.06
0.045
  23. BD (   1) C  10 - N  11        /***. BD*(   1) B  14 - B  15          0.83    1.21
0.028
  23. BD (   1) C  10 - N  11        /***. BD*(   1) C  41 - C  46          0.70    1.36
0.028
  23. BD (   1) C  10 - N  11        /***. BD*(   2) C  41 - C  46          0.76    0.75
0.023
  24. BD (   1) C  10 - B  14        /338. RY*(   1) N   9                  0.63    1.37
0.026
  24. BD (   1) C  10 - B  14        /339. RY*(   2) N   9                  0.84    1.91
0.036
  24. BD (   1) C  10 - B  14        /366. RY*(   1) N  11                  0.51    1.32
0.023
  24. BD (   1) C  10 - B  14        /367. RY*(   2) N  11                  1.13    1.95
0.042
  24. BD (   1) C  10 - B  14        /411. RY*(   4) B  14                  0.56    1.73
0.028
  24. BD (   1) C  10 - B  14        /413. RY*(   6) B  14                  0.96    3.97
0.056
  24. BD (   1) C  10 - B  14        /414. RY*(   7) B  14                  0.62    3.05
0.039
  24. BD (   1) C  10 - B  14        /416. RY*(   9) B  14                  1.14    4.98
0.068
  24. BD (   1) C  10 - B  14        /419. RY*(  12) B  14                  0.55    4.69
0.046
  24. BD (   1) C  10 - B  14        /422. RY*(   1) B  15                  2.95    2.14
0.072
  24. BD (   1) C  10 - B  14        /***. BD*(   1) C   1 - B  14          0.93    0.85
0.026
  24. BD (   1) C  10 - B  14        /***. BD*(   1) C   1 - B  15          1.42    0.96
0.033
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  24. BD (   1) C  10 - B  14        /***. BD*(   1) N   9 - C  10           1.57    0.86
0.033
  24. BD (   1) C  10 - B  14        /***. BD*(   1) N   9 - C  13           3.46    0.86
0.049
  24. BD (   1) C  10 - B  14        /***. BD*(   1) C  10 - N  11           1.51    0.86
0.032
  24. BD (   1) C  10 - B  14        /***. BD*(   1) N  11 - C  12           3.34    0.85
0.048
  24. BD (   1) C  10 - B  14        /***. BD*(   1) B  14 - B  15           3.14    1.00
0.050
  24. BD (   1) C  10 - B  14        /***. BD*(   1) B  15 - C  16           0.95    0.92
0.027
  25. BD (   1) N  11 - C  12        /352. RY*(   1) C  10                  0.75    2.36
0.038
  25. BD (   1) N  11 - C  12        /354. RY*(   3) C  10                  0.91    2.39
0.042
  25. BD (   1) N  11 - C  12        /396. RY*(   3) C  13                  0.86    1.78
0.035
  25. BD (   1) N  11 - C  12        /787. RY*(   2) C  41                  0.67    1.50
0.028
  25. BD (   1) N  11 - C  12        /***. BD*(   1) C   4 - N   9          0.69    1.03
0.024
  25. BD (   1) N  11 - C  12        /***. BD*(   1) N   9 - C  10          0.67    1.07
0.024
  25. BD (   1) N  11 - C  12        /***. BD*(   1) C  10 - N  11          0.86    1.06
0.027
  25. BD (   1) N  11 - C  12        /***. BD*(   1) C  10 - B  14          2.99    1.16
0.053
  25. BD (   1) N  11 - C  12        /***. BD*(   1) N  11 - C  41          0.84    1.02
0.026
  25. BD (   1) N  11 - C  12        /***. BD*(   1) C  12 - C  13          0.67    1.22
0.026
  25. BD (   1) N  11 - C  12        /***. BD*(   1) C  13 - H  72          3.68    1.05
0.056
  25. BD (   1) N  11 - C  12        /***. BD*(   1) C  41 - C  42          0.90    1.35
0.031
  25. BD (   1) N  11 - C  12        /***. BD*(   2) C  41 - C  46          1.34    0.74
0.031
  26. BD (   1) N  11 - C  41        /352. RY*(   1) C  10                  0.82    2.35
0.039
  26. BD (   1) N  11 - C  41        /381. RY*(   2) C  12                  0.65    2.04
0.033
  26. BD (   1) N  11 - C  41        /799. RY*(   1) C  42                  0.70    2.08
0.034
  26. BD (   1) N  11 - C  41        /855. RY*(   1) C  46                  0.61    2.10
0.032
  26. BD (   1) N  11 - C  41        /***. BD*(   1) N   9 - C  10          1.27    1.06
0.033
  26. BD (   1) N  11 - C  41        /***. BD*(   1) C  10 - N  11          0.89    1.06
0.027
  26. BD (   1) N  11 - C  41        /***. BD*(   1) N  11 - C  12          0.56    1.05
0.022
  26. BD (   1) N  11 - C  41        /***. BD*(   2) N  11 - C  41          0.67    1.70
0.034
  26. BD (   1) N  11 - C  41        /***. BD*(   1) C  12 - C  13          0.91    1.21
0.030
  26. BD (   1) N  11 - C  41        /***. BD*(   1) C  41 - C  46          0.67    1.35
0.027
  26. BD (   1) N  11 - C  41        /***. BD*(   1) C  42 - C  43          2.42    1.19
0.048
  26. BD (   1) N  11 - C  41        /***. BD*(   1) C  45 - C  46          2.26    1.18
0.046
  27. BD (   2) N  11 - C  41        /358. RY*(   7) C  10                  1.13    2.14
0.049
  27. BD (   2) N  11 - C  41        /380. RY*(   1) C  12                  2.89    0.90
0.051
  27. BD (   2) N  11 - C  41        /788. RY*(   3) C  41                  0.73    1.70
0.035
  27. BD (   2) N  11 - C  41        /794. RY*(   9) C  41                  0.94    2.03
0.043
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  27. BD (   2) N  11 - C  41        /***. BD*(   2) N   9 - C  10           43.76    0.18
0.088
  27. BD (   2) N  11 - C  41        /***. BD*(   2) N  11 - C  41            2.99    1.23
0.055
  27. BD (   2) N  11 - C  41        /***. BD*(   2) C  12 - C  13           26.04    0.22
0.069
  27. BD (   2) N  11 - C  41        /***. BD*(   1) C  41 - C  42            7.56    0.87
0.080
  27. BD (   2) N  11 - C  41        /***. BD*(   1) C  41 - C  46            7.71    0.87
0.081
  27. BD (   2) N  11 - C  41        /***. BD*(   2) C  41 - C  46            1.66    0.26
0.018
  27. BD (   2) N  11 - C  41        /***. BD*(   1) C  42 - C  43            0.65    0.71
0.021
  27. BD (   2) N  11 - C  41        /***. BD*(   1) C  45 - C  46            0.66    0.70
0.021
  28. BD (   1) C  12 - C  13        /339. RY*(   2) N   9                   1.28    2.06
0.046
  28. BD (   1) C  12 - C  13        /367. RY*(   2) N  11                   1.33    2.11
0.047
  28. BD (   1) C  12 - C  13        /***. BD*(   1) C   4 - N   9           5.06    0.98
0.063
  28. BD (   1) C  12 - C  13        /***. BD*(   1) N  11 - C  41           4.94    0.98
0.062
  28. BD (   1) C  12 - C  13        /***. BD*(   1) C  12 - H  71           0.98    1.00
0.028
  28. BD (   1) C  12 - C  13        /***. BD*(   1) C  13 - H  72           0.99    1.00
0.028
  29. BD (   2) C  12 - C  13        /***. BD*(   2) N   9 - C  10           6.33    0.20
0.039
  30. BD (   1) C  12 - H  71        /367. RY*(   2) N  11                   1.20    1.94
0.043
  30. BD (   1) C  12 - H  71        /395. RY*(   2) C  13                   0.98    1.83
0.038
  30. BD (   1) C  12 - H  71        /***. BD*(   1) N   9 - C  13           2.04    0.84
0.037
  30. BD (   1) C  12 - H  71        /***. BD*(   1) C  10 - N  11           3.90    0.85
0.052
  30. BD (   1) C  12 - H  71        /***. BD*(   1) C  12 - C  13           0.83    1.00
0.026
  31. BD (   1) C  13 - H  72        /339. RY*(   2) N   9                   1.12    1.89
0.041
  31. BD (   1) C  13 - H  72        /381. RY*(   2) C  12                   1.01    1.84
0.039
  31. BD (   1) C  13 - H  72        /***. BD*(   1) N   9 - C  10           3.91    0.85
0.052
  31. BD (   1) C  13 - H  72        /***. BD*(   1) N  11 - C  12           2.06    0.84
0.037
  31. BD (   1) C  13 - H  72        /***. BD*(   1) C  12 - C  13           0.84    1.00
0.026
  32. BD (   1) B  14 - B  15        /226. RY*(   1) C   1                   0.81    1.30
0.030
  32. BD (   1) B  14 - B  15        /352. RY*(   1) C  10                   2.17    1.93
0.060
  32. BD (   1) B  14 - B  15        /355. RY*(   4) C  10                   1.11    1.88
0.043
  32. BD (   1) B  14 - B  15        /356. RY*(   5) C  10                   0.74    1.36
0.030
  32. BD (   1) B  14 - B  15        /408. RY*(   1) B  14                   1.57    1.80
0.050
  32. BD (   1) B  14 - B  15        /411. RY*(   4) B  14                   0.52    1.50
0.026
  32. BD (   1) B  14 - B  15        /419. RY*(  12) B  14                   0.66    4.47
0.051
  32. BD (   1) B  14 - B  15        /422. RY*(   1) B  15                   0.54    1.92
0.030
  32. BD (   1) B  14 - B  15        /432. RY*(  11) B  15                   0.66    3.34
0.044
  32. BD (   1) B  14 - B  15        /436. RY*(   1) C  16                   1.89    2.11
0.059
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  32. BD (   1) B  14 - B  15        /438. RY*(   3) C  16                  0.51    1.74
0.028
  32. BD (   1) B  14 - B  15        /***. BD*(   1) C   1 - O   2          22.95    0.80
0.125
  32. BD (   1) B  14 - B  15        /***. BD*(   1) C   1 - B  14           2.81    0.62
0.038
  32. BD (   1) B  14 - B  15        /***. BD*(   1) C   1 - B  15           2.60    0.74
0.040
  32. BD (   1) B  14 - B  15        /***. BD*(   1) N   9 - C  10           1.02    0.64
0.024
  32. BD (   1) B  14 - B  15        /***. BD*(   2) N   9 - C  10           0.98    0.24
0.016
  32. BD (   1) B  14 - B  15        /***. BD*(   1) C  10 - N  11           1.40    0.64
0.027
  32. BD (   1) B  14 - B  15        /***. BD*(   1) C  10 - B  14           1.88    0.73
0.034
  32. BD (   1) B  14 - B  15        /***. BD*(   1) B  15 - C  16           3.67    0.70
0.047
  32. BD (   1) B  14 - B  15        /***. BD*(   1) C  16 - N  17           3.97    0.64
0.047
  33. BD (   1) B  15 - C  16        /408. RY*(   1) B  14                  2.55    2.03
0.065
  33. BD (   1) B  15 - C  16        /430. RY*(   9) B  15                  1.21    6.96
0.083
  33. BD (   1) B  15 - C  16        /433. RY*(  12) B  15                  0.74    4.49
0.052
  33. BD (   1) B  15 - C  16        /436. RY*(   1) C  16                  0.70    2.33
0.036
  33. BD (   1) B  15 - C  16        /450. RY*(   1) N  17                  1.55    1.99
0.050
  33. BD (   1) B  15 - C  16        /452. RY*(   3) N  17                  0.56    1.46
0.026
  33. BD (   1) B  15 - C  16        /492. RY*(   1) N  20                  1.50    1.90
0.048
  33. BD (   1) B  15 - C  16        /***. BD*(   1) C   1 - O   2          1.60    1.02
0.036
  33. BD (   1) B  15 - C  16        /***. BD*(   1) C   1 - B  14          1.35    0.84
0.031
  33. BD (   1) B  15 - C  16        /***. BD*(   1) C   1 - B  15          2.45    0.96
0.044
  33. BD (   1) B  15 - C  16        /***. BD*(   1) C  10 - B  14          1.75    0.95
0.036
  33. BD (   1) B  15 - C  16        /***. BD*(   1) B  14 - B  15          4.92    0.99
0.062
  33. BD (   1) B  15 - C  16        /***. BD*(   1) C  16 - N  17          1.35    0.86
0.031
  33. BD (   1) B  15 - C  16        /***. BD*(   1) C  16 - N  20          1.36    0.86
0.031
  33. BD (   1) B  15 - C  16        /***. BD*(   1) N  17 - C  18          3.77    0.84
0.050
  33. BD (   1) B  15 - C  16        /***. BD*(   1) C  19 - N  20          3.63    0.84
0.049
  34. BD (   1) C  16 - N  17        /466. RY*(   3) C  18                  0.68    1.86
0.032
  34. BD (   1) C  16 - N  17        /492. RY*(   1) N  20                  0.64    2.14
0.033
  34. BD (   1) C  16 - N  17        /507. RY*(   2) C  21                  0.76    1.50
0.030
  34. BD (   1) C  16 - N  17        /***. BD*(   1) B  14 - B  15          0.92    1.23
0.030
  34. BD (   1) C  16 - N  17        /***. BD*(   1) B  15 - C  16          1.68    1.16
0.040
  34. BD (   1) C  16 - N  17        /***. BD*(   1) N  17 - C  18          1.08    1.08
0.031
  34. BD (   1) C  16 - N  17        /***. BD*(   1) N  17 - C  21          1.05    1.04
0.030
  34. BD (   1) C  16 - N  17        /***. BD*(   1) C  18 - H  63          2.43    1.07
0.046
  34. BD (   1) C  16 - N  17        /***. BD*(   1) N  20 - C  31          5.14    1.04
0.065
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  34. BD (   1) C  16 - N  17        /***. BD*(   1) C  21 - C  22            0.56    1.20
0.023
  34. BD (   1) C  16 - N  17        /***. BD*(   1) C  21 - C  26            0.71    1.20
0.026
  34. BD (   1) C  16 - N  17        /***. BD*(   2) C  21 - C  26            0.73    0.75
0.023
  35. BD (   2) C  16 - N  17        /224. LP (   1) B  15                   3.98    0.34
0.039
  35. BD (   2) C  16 - N  17        /464. RY*(   1) C  18                   2.06    0.93
0.041
  35. BD (   2) C  16 - N  17        /508. RY*(   3) C  21                   1.11    1.29
0.035
  35. BD (   2) C  16 - N  17        /***. BD*(   2) C  18 - C  19           16.05    0.28
0.062
  35. BD (   2) C  16 - N  17        /***. BD*(   1) C  21 - C  22            3.67    0.77
0.049
  35. BD (   2) C  16 - N  17        /***. BD*(   1) C  21 - C  26            3.63    0.77
0.048
  36. BD (   1) C  16 - N  20        /450. RY*(   1) N  17                   0.63    2.23
0.034
  36. BD (   1) C  16 - N  20        /480. RY*(   3) C  19                   0.68    1.84
0.032
  36. BD (   1) C  16 - N  20        /647. RY*(   2) C  31                   0.92    1.49
0.033
  36. BD (   1) C  16 - N  20        /***. BD*(   1) B  15 - C  16           1.63    1.16
0.039
  36. BD (   1) C  16 - N  20        /***. BD*(   1) N  17 - C  21           5.05    1.04
0.065
  36. BD (   1) C  16 - N  20        /***. BD*(   1) C  19 - N  20           1.10    1.08
0.031
  36. BD (   1) C  16 - N  20        /***. BD*(   1) C  19 - H  64           2.33    1.07
0.045
  36. BD (   1) C  16 - N  20        /***. BD*(   1) N  20 - C  31           1.08    1.04
0.030
  36. BD (   1) C  16 - N  20        /***. BD*(   1) C  31 - C  32           0.68    1.20
0.026
  36. BD (   1) C  16 - N  20        /***. BD*(   1) C  31 - C  36           0.56    1.20
0.023
  36. BD (   1) C  16 - N  20        /***. BD*(   2) C  31 - C  36           0.80    0.75
0.024
  37. BD (   1) N  17 - C  18        /436. RY*(   1) C  16                   0.83    2.56
0.041
  37. BD (   1) N  17 - C  18        /439. RY*(   4) C  16                   1.41    2.26
0.051
  37. BD (   1) N  17 - C  18        /480. RY*(   3) C  19                   0.82    1.83
0.035
  37. BD (   1) N  17 - C  18        /507. RY*(   2) C  21                   0.65    1.50
0.028
  37. BD (   1) N  17 - C  18        /***. BD*(   1) B  15 - C  16           2.90    1.15
0.052
  37. BD (   1) N  17 - C  18        /***. BD*(   1) C  16 - N  17           0.94    1.10
0.029
  37. BD (   1) N  17 - C  18        /***. BD*(   1) C  16 - N  20           0.64    1.10
0.024
  37. BD (   1) N  17 - C  18        /***. BD*(   1) N  17 - C  21           0.85    1.03
0.027
  37. BD (   1) N  17 - C  18        /***. BD*(   1) C  18 - C  19           0.62    1.22
0.025
  37. BD (   1) N  17 - C  18        /***. BD*(   1) C  19 - H  64           3.51    1.06
0.055
  37. BD (   1) N  17 - C  18        /***. BD*(   1) N  20 - C  31           0.73    1.03
0.025
  37. BD (   1) N  17 - C  18        /***. BD*(   1) C  21 - C  22           0.84    1.20
0.028
  37. BD (   1) N  17 - C  18        /***. BD*(   2) C  21 - C  26           1.19    0.75
0.030
  38. BD (   1) N  17 - C  21        /436. RY*(   1) C  16                   1.04    2.54
0.046
  38. BD (   1) N  17 - C  21        /465. RY*(   2) C  18                   0.64    2.05
0.032
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  38. BD (   1) N  17 - C  21        /520. RY*(   1) C  22                  0.64    2.01
0.032
  38. BD (   1) N  17 - C  21        /576. RY*(   1) C  26                  0.56    2.12
0.031
  38. BD (   1) N  17 - C  21        /***. BD*(   1) C  16 - N  17          1.04    1.07
0.030
  38. BD (   1) N  17 - C  21        /***. BD*(   1) C  16 - N  20          1.51    1.07
0.036
  38. BD (   1) N  17 - C  21        /***. BD*(   1) N  17 - C  18          0.59    1.05
0.022
  38. BD (   1) N  17 - C  21        /***. BD*(   1) C  18 - C  19          0.92    1.19
0.030
  38. BD (   1) N  17 - C  21        /***. BD*(   1) C  21 - C  22          0.54    1.17
0.022
  38. BD (   1) N  17 - C  21        /***. BD*(   1) C  22 - C  23          2.32    1.20
0.047
  38. BD (   1) N  17 - C  21        /***. BD*(   1) C  25 - C  26          2.29    1.19
0.047
  39. BD (   1) C  18 - C  19        /450. RY*(   1) N  17                  1.26    2.16
0.047
  39. BD (   1) C  18 - C  19        /492. RY*(   1) N  20                  1.09    2.07
0.043
  39. BD (   1) C  18 - C  19        /***. BD*(   1) N  17 - C  21          5.20    0.97
0.064
  39. BD (   1) C  18 - C  19        /***. BD*(   1) C  18 - H  63          0.88    1.00
0.027
  39. BD (   1) C  18 - C  19        /***. BD*(   1) C  19 - H  64          0.90    1.00
0.027
  39. BD (   1) C  18 - C  19        /***. BD*(   1) N  20 - C  31          5.10    0.97
0.063
  40. BD (   2) C  18 - C  19        /***. BD*(   2) C  16 - N  17          7.87    0.21
0.041
  41. BD (   1) C  18 - H  63        /450. RY*(   1) N  17                  1.19    1.99
0.044
  41. BD (   1) C  18 - H  63        /479. RY*(   2) C  19                  0.98    1.80
0.038
  41. BD (   1) C  18 - H  63        /***. BD*(   1) C  16 - N  17          4.06    0.87
0.053
  41. BD (   1) C  18 - H  63        /***. BD*(   1) C  18 - C  19          0.71    0.99
0.024
  41. BD (   1) C  18 - H  63        /***. BD*(   1) C  19 - N  20          1.88    0.84
0.036
  42. BD (   1) C  19 - N  20        /436. RY*(   1) C  16                  0.85    2.56
0.042
  42. BD (   1) C  19 - N  20        /438. RY*(   3) C  16                  0.78    2.19
0.037
  42. BD (   1) C  19 - N  20        /466. RY*(   3) C  18                  0.80    1.85
0.035
  42. BD (   1) C  19 - N  20        /647. RY*(   2) C  31                  0.67    1.48
0.028
  42. BD (   1) C  19 - N  20        /***. BD*(   1) B  15 - C  16          2.97    1.15
0.053
  42. BD (   1) C  19 - N  20        /***. BD*(   1) C  16 - N  17          0.65    1.10
0.024
  42. BD (   1) C  19 - N  20        /***. BD*(   1) C  16 - N  20          0.96    1.10
0.029
  42. BD (   1) C  19 - N  20        /***. BD*(   1) N  17 - C  21          0.73    1.03
0.025
  42. BD (   1) C  19 - N  20        /***. BD*(   1) C  18 - C  19          0.60    1.22
0.024
  42. BD (   1) C  19 - N  20        /***. BD*(   1) C  18 - H  63          3.54    1.06
0.055
  42. BD (   1) C  19 - N  20        /***. BD*(   1) N  20 - C  31          0.82    1.03
0.026
  42. BD (   1) C  19 - N  20        /***. BD*(   1) C  31 - C  36          0.80    1.19
0.028
  42. BD (   1) C  19 - N  20        /***. BD*(   2) C  31 - C  36          1.25    0.74
0.030
  43. BD (   1) C  19 - H  64        /465. RY*(   2) C  18                  0.99    1.85
0.038
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43. BD (1) C 19 - H 64 /492. RY*(1) N 20 1.09 1.90
0.041
43. BD (1) C 19 - H 64 /***. BD*(1) C 16 - N 20 4.07 0.87
0.053
43. BD (1) C 19 - H 64 /***. BD*(1) N 17 - C 18 1.91 0.85
0.036
43. BD (1) C 19 - H 64 /***. BD*(1) C 18 - C 19 0.73 0.99
0.024
44. BD (1) N 20 - C 31 /436. RY*(1) C 16 0.96 2.55
0.044
44. BD (1) N 20 - C 31 /479. RY*(2) C 19 0.63 2.01
0.032
44. BD (1) N 20 - C 31 /660. RY*(1) C 32 0.56 2.13
0.031
44. BD (1) N 20 - C 31 /716. RY*(1) C 36 0.59 2.11
0.032
44. BD (1) N 20 - C 31 /***. BD*(1) C 16 - N 17 1.44 1.08
0.035
44. BD (1) N 20 - C 31 /***. BD*(1) C 16 - N 20 1.04 1.08
0.030
44. BD (1) N 20 - C 31 /***. BD*(1) C 18 - C 19 0.87 1.20
0.029
44. BD (1) N 20 - C 31 /***. BD*(1) C 19 - N 20 0.57 1.05
0.022
44. BD (1) N 20 - C 31 /***. BD*(1) C 31 - C 32 0.51 1.17
0.022
44. BD (1) N 20 - C 31 /***. BD*(1) C 31 - C 36 0.56 1.18
0.023
44. BD (1) N 20 - C 31 /***. BD*(1) C 32 - C 33 2.23 1.19
0.046
44. BD (1) N 20 - C 31 /***. BD*(1) C 35 - C 36 2.31 1.19
0.047
45. BD (1) C 21 - C 22 /451. RY*(2) N 17 0.69 1.38
0.028
45. BD (1) C 21 - C 22 /578. RY*(3) C 26 0.71 1.69
0.031
45. BD (1) C 21 - C 22 /***. BD*(1) C 16 - N 17 1.41 0.98
0.033
45. BD (1) C 21 - C 22 /***. BD*(2) C 16 - N 17 0.66 0.57
0.021
45. BD (1) C 21 - C 22 /***. BD*(1) N 17 - C 18 1.14 0.97
0.030
45. BD (1) C 21 - C 22 /***. BD*(1) C 21 - C 26 2.47 1.09
0.046
45. BD (1) C 21 - C 22 /***. BD*(1) C 22 - C 23 1.25 1.11
0.033
45. BD (1) C 21 - C 22 /***. BD*(1) C 22 - C 27 0.59 0.96
0.021
45. BD (1) C 21 - C 22 /***. BD*(1) C 23 - H 67 2.86 0.99
0.048
45. BD (1) C 21 - C 22 /***. BD*(1) C 26 - C 29 3.76 0.95
0.053
45. BD (1) C 21 - C 22 /***. BD*(1) C 27 - C 62 1.13 0.93
0.029
46. BD (1) C 21 - C 26 /451. RY*(2) N 17 0.89 1.38
0.031
46. BD (1) C 21 - C 26 /522. RY*(3) C 22 0.79 1.60
0.032
46. BD (1) C 21 - C 26 /***. BD*(1) C 16 - N 17 1.69 0.99
0.037
46. BD (1) C 21 - C 26 /***. BD*(2) C 16 - N 17 0.86 0.58
0.024
46. BD (1) C 21 - C 26 /***. BD*(1) N 17 - C 18 0.74 0.97
0.024
46. BD (1) C 21 - C 26 /***. BD*(1) C 21 - C 22 2.48 1.09
0.046
46. BD (1) C 21 - C 26 /***. BD*(1) C 22 - C 27 3.62 0.97
0.053
46. BD (1) C 21 - C 26 /***. BD*(1) C 25 - C 26 1.41 1.10
0.035

46. BD (1) C 21 - C 26 /***. BD*(1) C 25 - H 65 2.85 0.98
0.047
46. BD (1) C 21 - C 26 /***. BD*(1) C 26 - C 29 0.63 0.96
0.022
46. BD (1) C 21 - C 26 /***. BD*(1) C 29 - C 30 0.60 0.92
0.021
46. BD (1) C 21 - C 26 /***. BD*(1) C 29 - C 61 0.59 0.92
0.021
47. BD (2) C 21 - C 26 /521. RY*(2) C 22 0.53 0.91
0.021
47. BD (2) C 21 - C 26 /564. RY*(3) C 25 1.37 0.80
0.032
47. BD (2) C 21 - C 26 /***. BD*(1) C 16 - N 17 3.22 0.58
0.042
47. BD (2) C 21 - C 26 /***. BD*(1) N 17 - C 18 3.05 0.56
0.040
47. BD (2) C 21 - C 26 /***. BD*(2) C 22 - C 23 16.25 0.24
0.056
47. BD (2) C 21 - C 26 /***. BD*(2) C 24 - C 25 13.12 0.23
0.049
47. BD (2) C 21 - C 26 /***. BD*(1) C 29 - C 30 2.13 0.51
0.032
47. BD (2) C 21 - C 26 /***. BD*(1) C 29 - C 61 2.20 0.51
0.033
48. BD (1) C 22 - C 23 /506. RY*(1) C 21 0.86 1.89
0.036
48. BD (1) C 22 - C 23 /549. RY*(2) C 24 0.97 1.83
0.038
48. BD (1) C 22 - C 23 /590. RY*(1) C 27 0.53 1.70
0.027
48. BD (1) C 22 - C 23 /***. BD*(1) N 17 - C 21 5.34 0.92
0.063
48. BD (1) C 22 - C 23 /***. BD*(1) C 21 - C 22 1.53 1.08
0.036
48. BD (1) C 22 - C 23 /***. BD*(1) C 22 - C 27 0.71 0.96
0.023
48. BD (1) C 22 - C 23 /***. BD*(1) C 23 - C 24 1.57 1.12
0.038
48. BD (1) C 22 - C 23 /***. BD*(1) C 24 - H 66 2.47 0.97
0.044
48. BD (1) C 22 - C 23 /***. BD*(1) C 27 - H 84 0.84 0.95
0.025
49. BD (2) C 22 - C 23 /550. RY*(3) C 24 0.68 0.79
0.023
49. BD (2) C 22 - C 23 /***. BD*(2) C 21 - C 26 14.54 0.22
0.051
49. BD (2) C 22 - C 23 /***. BD*(2) C 24 - C 25 16.49 0.22
0.054
49. BD (2) C 22 - C 23 /***. BD*(1) C 27 - C 28 2.60 0.50
0.036
49. BD (2) C 22 - C 23 /***. BD*(1) C 27 - C 62 0.67 0.52
0.018
49. BD (2) C 22 - C 23 /***. BD*(1) C 27 - H 84 0.77 0.54
0.020
50. BD (1) C 22 - C 27 /506. RY*(1) C 21 1.41 1.81
0.045
50. BD (1) C 22 - C 27 /534. RY*(1) C 23 0.87 1.98
0.037
50. BD (1) C 22 - C 27 /***. BD*(1) C 21 - C 22 0.73 1.00
0.024
50. BD (1) C 22 - C 27 /***. BD*(1) C 21 - C 26 3.95 1.00
0.056
50. BD (1) C 22 - C 27 /***. BD*(1) C 22 - C 23 0.77 1.03
0.025
50. BD (1) C 22 - C 27 /***. BD*(1) C 23 - C 24 2.75 1.04
0.048
50. BD (1) C 22 - C 27 /***. BD*(1) C 28 - H 90 1.50 0.87
0.032
50. BD (1) C 22 - C 27 /***. BD*(1) C 62 - H 87 1.24 0.88
0.030

51. BD (1) C 23 - C 24 /520. RY*(1) C 22 1.26 1.93
0.044
51. BD (1) C 23 - C 24 /563. RY*(2) C 25 0.71 1.73
0.031
51. BD (1) C 23 - C 24 /***. BD*(1) C 22 - C 23 1.81 1.11
0.040
51. BD (1) C 23 - C 24 /***. BD*(1) C 22 - C 27 4.11 0.96
0.056
51. BD (1) C 23 - C 24 /***. BD*(1) C 24 - C 25 1.48 1.12
0.036
51. BD (1) C 23 - C 24 /***. BD*(1) C 25 - H 65 2.67 0.98
0.046
52. BD (1) C 23 - H 67 /520. RY*(1) C 22 1.59 1.75
0.047
52. BD (1) C 23 - H 67 /548. RY*(1) C 24 0.99 1.67
0.037
52. BD (1) C 23 - H 67 /***. BD*(1) C 21 - C 22 5.24 0.91
0.062
52. BD (1) C 23 - H 67 /***. BD*(1) C 24 - C 25 3.93 0.94
0.054
53. BD (1) C 24 - C 25 /534. RY*(1) C 23 0.51 2.06
0.029
53. BD (1) C 24 - C 25 /535. RY*(2) C 23 0.53 1.49
0.025
53. BD (1) C 24 - C 25 /576. RY*(1) C 26 1.39 2.04
0.048
53. BD (1) C 24 - C 25 /***. BD*(1) C 23 - C 24 1.46 1.13
0.036
53. BD (1) C 24 - C 25 /***. BD*(1) C 23 - H 67 2.51 0.99
0.044
53. BD (1) C 24 - C 25 /***. BD*(1) C 25 - C 26 1.81 1.11
0.040
53. BD (1) C 24 - C 25 /***. BD*(1) C 26 - C 29 4.04 0.96
0.056
54. BD (2) C 24 - C 25 /***. BD*(2) C 21 - C 26 16.61 0.23
0.056
54. BD (2) C 24 - C 25 /***. BD*(2) C 22 - C 23 13.26 0.24
0.050
55. BD (1) C 24 - H 66 /534. RY*(1) C 23 1.41 1.88
0.046
55. BD (1) C 24 - H 66 /562. RY*(1) C 25 1.41 1.88
0.046
55. BD (1) C 24 - H 66 /***. RY*(1) H 65 0.52 1.07
0.021
55. BD (1) C 24 - H 66 /***. RY*(1) H 67 0.52 1.08
0.021
55. BD (1) C 24 - H 66 /***. BD*(1) C 22 - C 23 4.52 0.93
0.058
55. BD (1) C 24 - H 66 /***. BD*(1) C 25 - C 26 4.54 0.92
0.058
56. BD (1) C 25 - C 26 /506. RY*(1) C 21 0.89 1.89
0.037
56. BD (1) C 25 - C 26 /549. RY*(2) C 24 0.92 1.84
0.037
56. BD (1) C 25 - C 26 /618. RY*(1) C 29 0.72 1.74
0.032
56. BD (1) C 25 - C 26 /***. BD*(1) N 17 - C 21 5.15 0.92
0.062
56. BD (1) C 25 - C 26 /***. BD*(1) C 21 - C 26 1.66 1.09
0.038
56. BD (1) C 25 - C 26 /***. BD*(1) C 24 - C 25 1.56 1.12
0.037
56. BD (1) C 25 - C 26 /***. BD*(1) C 24 - H 66 2.53 0.98
0.044
56. BD (1) C 25 - C 26 /***. BD*(1) C 26 - C 29 0.71 0.95
0.023
56. BD (1) C 25 - C 26 /***. BD*(1) C 29 - H 83 1.07 0.94
0.028
57. BD (1) C 25 - H 65 /548. RY*(1) C 24 1.00 1.68
0.037

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  57. BD (   1) C  25 - H  65        /576. RY*(   1) C  26                1.63    1.86
0.049
  57. BD (   1) C  25 - H  65        /***. BD*(   1) C  21 - C  26        5.28    0.91
0.062
  57. BD (   1) C  25 - H  65        /***. BD*(   1) C  23 - C  24        3.84    0.95
0.054
  58. BD (   1) C  26 - C  29        /506. RY*(   1) C  21                1.45    1.81
0.046
  58. BD (   1) C  26 - C  29        /562. RY*(   1) C  25                0.90    1.98
0.038
  58. BD (   1) C  26 - C  29        /***. BD*(   1) C  21 - C  22        3.78    1.01
0.055
  58. BD (   1) C  26 - C  29        /***. BD*(   1) C  21 - C  26        0.76    1.01
0.025
  58. BD (   1) C  26 - C  29        /***. BD*(   1) C  24 - C  25        2.73    1.04
0.048
  58. BD (   1) C  26 - C  29        /***. BD*(   1) C  25 - C  26        0.77    1.02
0.025
  58. BD (   1) C  26 - C  29        /***. BD*(   1) C  30 - H  93        1.42    0.87
0.032
  58. BD (   1) C  26 - C  29        /***. BD*(   1) C  61 - H  96        1.41    0.88
0.032
  59. BD (   1) C  27 - C  28        /521. RY*(   2) C  22                0.63    1.21
0.025
  59. BD (   1) C  27 - C  28        /***. RY*(   1) C  62                0.53    1.34
0.024
  59. BD (   1) C  27 - C  28        /***. BD*(   1) C  21 - C  22        0.96    0.98
0.028
  59. BD (   1) C  27 - C  28        /***. BD*(   1) C  22 - C  23        0.79    1.01
0.025
  59. BD (   1) C  27 - C  28        /***. BD*(   2) C  22 - C  23        2.92    0.54
0.038
  59. BD (   1) C  27 - C  28        /***. BD*(   1) C  62 - H  89        1.46    0.90
0.032
  60. BD (   1) C  27 - C  62        /***. BD*(   1) C  21 - C  22        3.47    0.98
0.052
  60. BD (   1) C  27 - C  62        /***. BD*(   2) C  22 - C  23        0.63    0.54
0.018
  60. BD (   1) C  27 - C  62        /***. BD*(   1) C  22 - C  27        0.62    0.86
0.021
  60. BD (   1) C  27 - C  62        /***. BD*(   1) C  28 - H  91        1.75    0.85
0.035
  61. BD (   1) C  27 - H  84        /***. BD*(   1) C  22 - C  23        4.48    0.89
0.057
  61. BD (   1) C  27 - H  84        /***. BD*(   2) C  22 - C  23        0.84    0.43
0.018
  61. BD (   1) C  27 - H  84        /***. BD*(   1) C  28 - H  92        2.73    0.73
0.040
  61. BD (   1) C  27 - H  84        /***. BD*(   1) C  62 - H  88        2.93    0.74
0.042
  62. BD (   1) C  28 - H  90        /***. BD*(   1) C  22 - C  27        3.24    0.77
0.045
  63. BD (   1) C  28 - H  91        /***. BD*(   1) C  27 - C  62        2.84    0.74
0.041
  64. BD (   1) C  28 - H  92        /***. BD*(   1) C  27 - H  84        2.34    0.76
0.038
  65. BD (   1) C  29 - C  30        /577. RY*(   2) C  26                0.83    1.33
0.030
  65. BD (   1) C  29 - C  30        /***. BD*(   1) C  21 - C  26        2.32    0.99
0.043
  65. BD (   1) C  29 - C  30        /***. BD*(   2) C  21 - C  26        2.00    0.55
0.033
  65. BD (   1) C  29 - C  30        /***. BD*(   1) C  26 - C  29        0.53    0.86
0.019
  65. BD (   1) C  29 - C  30        /***. BD*(   1) C  61 - H  97        1.54    0.89
0.033
  66. BD (   1) C  29 - C  61        /***. BD*(   1) C  21 - C  26        2.28    0.99
0.043
  66. BD (   1) C  29 - C  61        /***. BD*(   2) C  21 - C  26        2.03    0.54
0.033
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66. BD (1) C 29 - C 61 /***. BD*(1) C 26 - C 29 0.58 0.86
0.020
66. BD (1) C 29 - C 61 /***. BD*(1) C 30 - H 95 1.66 0.85
0.034
67. BD (1) C 29 - H 83 /***. BD*(1) C 25 - C 26 4.77 0.90
0.059
67. BD (1) C 29 - H 83 /***. BD*(1) C 30 - H 94 2.79 0.74
0.041
67. BD (1) C 29 - H 83 /***. BD*(1) C 61 - H 98 2.80 0.75
0.041
68. BD (1) C 30 - H 93 /***. BD*(1) C 26 - C 29 3.34 0.76
0.045
69. BD (1) C 30 - H 94 /***. BD*(1) C 29 - H 83 2.25 0.76
0.037
70. BD (1) C 30 - H 95 /***. BD*(1) C 29 - C 61 3.10 0.73
0.042
71. BD (1) C 31 - C 32 /493. RY*(2) N 20 0.68 1.48
0.029
71. BD (1) C 31 - C 32 /717. RY*(2) C 36 0.85 1.76
0.035
71. BD (1) C 31 - C 32 /***. BD*(1) C 16 - N 20 1.63 0.99
0.036
71. BD (1) C 31 - C 32 /***. BD*(1) C 19 - N 20 0.74 0.97
0.024
71. BD (1) C 31 - C 32 /***. BD*(1) C 31 - C 36 2.43 1.09
0.046
71. BD (1) C 31 - C 32 /***. BD*(1) C 32 - C 33 1.33 1.10
0.034
71. BD (1) C 31 - C 32 /***. BD*(1) C 32 - C 37 0.59 0.96
0.021
71. BD (1) C 31 - C 32 /***. BD*(1) C 33 - H 70 2.86 0.98
0.047
71. BD (1) C 31 - C 32 /***. BD*(1) C 36 - C 39 3.62 0.96
0.053
71. BD (1) C 31 - C 32 /***. BD*(1) C 37 - C 38 0.79 0.92
0.024
72. BD (1) C 31 - C 36 /493. RY*(2) N 20 0.64 1.48
0.028
72. BD (1) C 31 - C 36 /661. RY*(2) C 32 0.58 1.57
0.027
72. BD (1) C 31 - C 36 /703. RY*(2) C 35 0.52 1.72
0.027
72. BD (1) C 31 - C 36 /***. BD*(1) C 16 - N 20 1.39 0.99
0.033
72. BD (1) C 31 - C 36 /***. BD*(1) C 19 - N 20 1.11 0.97
0.029
72. BD (1) C 31 - C 36 /***. BD*(1) C 31 - C 32 2.41 1.09
0.046
72. BD (1) C 31 - C 36 /***. BD*(1) C 32 - C 37 3.59 0.96
0.052
72. BD (1) C 31 - C 36 /***. BD*(1) C 35 - C 36 1.33 1.11
0.034
72. BD (1) C 31 - C 36 /***. BD*(1) C 35 - H 68 2.86 0.98
0.048
72. BD (1) C 31 - C 36 /***. BD*(1) C 36 - C 39 0.61 0.96
0.022
72. BD (1) C 31 - C 36 /***. BD*(1) C 39 - C 40 0.52 0.92
0.020
72. BD (1) C 31 - C 36 /***. BD*(1) C 39 - C 56 0.66 0.94
0.022
73. BD (2) C 31 - C 36 /704. RY*(3) C 35 1.25 0.81
0.031
73. BD (2) C 31 - C 36 /***. BD*(1) C 16 - N 20 3.20 0.59
0.042
73. BD (2) C 31 - C 36 /***. BD*(1) C 19 - N 20 3.15 0.56
0.041
73. BD (2) C 31 - C 36 /***. BD*(2) C 32 - C 33 16.93 0.23
0.056
73. BD (2) C 31 - C 36 /***. BD*(2) C 34 - C 35 13.39 0.23
0.050

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  73. BD (   2) C  31 - C  36        /***. BD*(   1) C  39 - C  40            2.20    0.51
0.033
  73. BD (   2) C  31 - C  36        /***. BD*(   1) C  39 - C  56            1.94    0.53
0.031
  74. BD (   1) C  32 - C  33        /646. RY*(   1) C  31                    0.83    1.95
0.036
  74. BD (   1) C  32 - C  33        /689. RY*(   2) C  34                    0.95    1.84
0.038
  74. BD (   1) C  32 - C  33        /730. RY*(   1) C  37                    0.73    1.75
0.032
  74. BD (   1) C  32 - C  33        /***. BD*(   1) N  20 - C  31            5.01    0.93
0.061
  74. BD (   1) C  32 - C  33        /***. BD*(   1) C  31 - C  32            1.55    1.08
0.037
  74. BD (   1) C  32 - C  33        /***. BD*(   1) C  32 - C  37            0.71    0.95
0.023
  74. BD (   1) C  32 - C  33        /***. BD*(   1) C  33 - C  34            1.55    1.12
0.037
  74. BD (   1) C  32 - C  33        /***. BD*(   1) C  34 - H  69            2.50    0.98
0.044
  74. BD (   1) C  32 - C  33        /***. BD*(   1) C  37 - H  85            1.00    0.95
0.027
  75. BD (   2) C  32 - C  33        /690. RY*(   3) C  34                    0.72    0.83
0.024
  75. BD (   2) C  32 - C  33        /***. BD*(   2) C  31 - C  36           14.02    0.23
0.051
  75. BD (   2) C  32 - C  33        /***. BD*(   2) C  34 - C  35           16.14    0.22
0.054
  75. BD (   2) C  32 - C  33        /***. BD*(   1) C  37 - C  38            1.38    0.51
0.026
  75. BD (   2) C  32 - C  33        /***. BD*(   1) C  37 - C  55            2.18    0.51
0.033
  76. BD (   1) C  32 - C  37        /646. RY*(   1) C  31                    1.54    1.87
0.048
  76. BD (   1) C  32 - C  37        /674. RY*(   1) C  33                    0.91    1.98
0.038
  76. BD (   1) C  32 - C  37        /***. BD*(   1) C  31 - C  32            0.72    1.01
0.024
  76. BD (   1) C  32 - C  37        /***. BD*(   1) C  31 - C  36            3.77    1.01
0.055
  76. BD (   1) C  32 - C  37        /***. BD*(   1) C  32 - C  33            0.77    1.02
0.025
  76. BD (   1) C  32 - C  37        /***. BD*(   1) C  33 - C  34            2.71    1.04
0.048
  76. BD (   1) C  32 - C  37        /***. BD*(   1) C  38 - H 105            1.33    0.88
0.031
  76. BD (   1) C  32 - C  37        /***. BD*(   1) C  55 - H 108            1.44    0.88
0.032
  77. BD (   1) C  33 - C  34        /660. RY*(   1) C  32                    1.35    2.04
0.047
  77. BD (   1) C  33 - C  34        /703. RY*(   2) C  35                    0.64    1.73
0.030
  77. BD (   1) C  33 - C  34        /***. BD*(   1) C  32 - C  33            1.79    1.11
0.040
  77. BD (   1) C  33 - C  34        /***. BD*(   1) C  32 - C  37            4.03    0.96
0.056
  77. BD (   1) C  33 - C  34        /***. BD*(   1) C  34 - C  35            1.49    1.12
0.037
  77. BD (   1) C  33 - C  34        /***. BD*(   1) C  35 - H  68            2.62    0.99
0.045
  78. BD (   1) C  33 - H  70        /660. RY*(   1) C  32                    1.66    1.86
0.050
  78. BD (   1) C  33 - H  70        /688. RY*(   1) C  34                    1.01    1.67
0.037
  78. BD (   1) C  33 - H  70        /***. BD*(   1) C  31 - C  32            5.16    0.91
0.061
  78. BD (   1) C  33 - H  70        /***. BD*(   1) C  34 - C  35            3.93    0.94
0.055
  79. BD (   1) C  34 - C  35        /716. RY*(   1) C  36                    1.41    2.03
0.048
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79. BD (1) C 34 - C 35	/***. BD*(1) C 33 - C 34	1.48	1.12	0.036
79. BD (1) C 34 - C 35	/***. BD*(1) C 33 - H 70	2.61	0.98	0.045
79. BD (1) C 34 - C 35	/***. BD*(1) C 35 - C 36	1.77	1.11	0.040
79. BD (1) C 34 - C 35	/***. BD*(1) C 36 - C 39	4.04	0.97	0.056
80. BD (2) C 34 - C 35	/***. BD*(2) C 31 - C 36	16.61	0.23	0.056
80. BD (2) C 34 - C 35	/***. BD*(2) C 32 - C 33	13.72	0.23	0.050
81. BD (1) C 34 - H 69	/674. RY*(1) C 33	1.41	1.88	0.046
81. BD (1) C 34 - H 69	/702. RY*(1) C 35	1.44	1.86	0.046
81. BD (1) C 34 - H 69	/***. RY*(1) H 68	0.51	1.08	0.021
81. BD (1) C 34 - H 69	/***. RY*(1) H 70	0.52	1.07	0.021
81. BD (1) C 34 - H 69	/***. BD*(1) C 32 - C 33	4.50	0.93	0.058
81. BD (1) C 34 - H 69	/***. BD*(1) C 35 - C 36	4.57	0.93	0.058
82. BD (1) C 35 - C 36	/646. RY*(1) C 31	0.86	1.95	0.037
82. BD (1) C 35 - C 36	/689. RY*(2) C 34	0.95	1.84	0.038
82. BD (1) C 35 - C 36	/758. RY*(1) C 39	0.72	1.75	0.032
82. BD (1) C 35 - C 36	/***. BD*(1) N 20 - C 31	5.12	0.93	0.062
82. BD (1) C 35 - C 36	/***. BD*(1) C 31 - C 36	1.57	1.09	0.037
82. BD (1) C 35 - C 36	/***. BD*(1) C 34 - C 35	1.54	1.12	0.037
82. BD (1) C 35 - C 36	/***. BD*(1) C 34 - H 69	2.54	0.98	0.045
82. BD (1) C 35 - C 36	/***. BD*(1) C 36 - C 39	0.73	0.96	0.024
82. BD (1) C 35 - C 36	/***. BD*(1) C 39 - H 86	0.98	0.95	0.027
83. BD (1) C 35 - H 68	/688. RY*(1) C 34	1.02	1.67	0.037
83. BD (1) C 35 - H 68	/716. RY*(1) C 36	1.68	1.85	0.050
83. BD (1) C 35 - H 68	/***. BD*(1) C 31 - C 36	5.24	0.91	0.062
83. BD (1) C 35 - H 68	/***. BD*(1) C 33 - C 34	3.97	0.94	0.055
84. BD (1) C 36 - C 39	/646. RY*(1) C 31	1.54	1.87	0.048
84. BD (1) C 36 - C 39	/702. RY*(1) C 35	0.90	1.95	0.038
84. BD (1) C 36 - C 39	/***. BD*(1) C 31 - C 32	3.85	1.00	0.056
84. BD (1) C 36 - C 39	/***. BD*(1) C 31 - C 36	0.75	1.01	0.025
84. BD (1) C 36 - C 39	/***. BD*(1) C 34 - C 35	2.78	1.04	0.048
84. BD (1) C 36 - C 39	/***. BD*(1) C 35 - C 36	0.79	1.02	0.025
84. BD (1) C 36 - C 39	/***. BD*(1) C 40 - H 99	1.42	0.88	0.032
84. BD (1) C 36 - C 39	/***. BD*(1) C 56 - H 102	1.36	0.89	0.031
85. BD (1) C 37 - C 38	/661. RY*(2) C 32	0.77	1.47	0.030
85. BD (1) C 37 - C 38	/***. BD*(1) C 31 - C 32	2.68	0.99	0.046

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  85. BD (   1) C  37 - C  38        /***. BD*(   2) C  32 - C  33           1.40    0.54
0.027
  85. BD (   1) C  37 - C  38        /***. BD*(   1) C  32 - C  37           0.53    0.86
0.019
  85. BD (   1) C  37 - C  38        /***. BD*(   1) C  55 - H 110           1.52    0.89
0.033
  86. BD (   1) C  37 - C  55        /662. RY*(   3) C  32                  0.60    1.42
0.026
  86. BD (   1) C  37 - C  55        /744. RY*(   1) C  38                  0.50    1.30
0.023
  86. BD (   1) C  37 - C  55        /***. BD*(   1) C  31 - C  32          1.75    0.98
0.037
  86. BD (   1) C  37 - C  55        /***. BD*(   2) C  32 - C  33          2.22    0.54
0.034
  86. BD (   1) C  37 - C  55        /***. BD*(   1) C  32 - C  37          0.56    0.85
0.020
  86. BD (   1) C  37 - C  55        /***. BD*(   1) C  38 - H 106          1.65    0.86
0.034
  87. BD (   1) C  37 - H  85        /***. BD*(   1) C  32 - C  33          4.76    0.89
0.058
  87. BD (   1) C  37 - H  85        /***. BD*(   1) C  38 - H 107          2.86    0.74
0.041
  87. BD (   1) C  37 - H  85        /***. BD*(   1) C  55 - H 109          2.77    0.75
0.041
  88. BD (   1) C  38 - H 105        /***. BD*(   1) C  32 - C  37          3.50    0.76
0.046
  89. BD (   1) C  38 - H 106        /***. BD*(   1) C  37 - C  55          3.11    0.73
0.043
  90. BD (   1) C  38 - H 107        /***. BD*(   1) C  37 - H  85          2.18    0.76
0.036
  91. BD (   1) C  39 - C  40        /718. RY*(   3) C  36                  0.84    1.32
0.030
  91. BD (   1) C  39 - C  40        /***. BD*(   1) C  31 - C  36          2.06    0.99
0.040
  91. BD (   1) C  39 - C  40        /***. BD*(   2) C  31 - C  36          2.33    0.54
0.035
  91. BD (   1) C  39 - C  40        /***. BD*(   1) C  36 - C  39          0.51    0.86
0.019
  91. BD (   1) C  39 - C  40        /***. BD*(   1) C  56 - H 103          1.51    0.89
0.033
  92. BD (   1) C  39 - C  56        /***. BD*(   1) C  31 - C  36          2.50    0.98
0.044
  92. BD (   1) C  39 - C  56        /***. BD*(   2) C  31 - C  36          1.85    0.53
0.031
  92. BD (   1) C  39 - C  56        /***. BD*(   1) C  36 - C  39          0.58    0.85
0.020
  92. BD (   1) C  39 - C  56        /***. BD*(   1) C  40 - H 101          1.64    0.85
0.034
  93. BD (   1) C  39 - H  86        /***. BD*(   1) C  35 - C  36          4.95    0.89
0.059
  93. BD (   1) C  39 - H  86        /***. BD*(   1) C  40 - H 100          2.79    0.74
0.041
  93. BD (   1) C  39 - H  86        /***. BD*(   1) C  56 - H 104          2.88    0.75
0.042
  94. BD (   1) C  40 - H  99        /***. BD*(   1) C  36 - C  39          3.30    0.76
0.045
  95. BD (   1) C  40 - H 100        /***. BD*(   1) C  39 - H  86          2.21    0.76
0.037
  96. BD (   1) C  40 - H 101        /***. BD*(   1) C  39 - C  56          3.04    0.74
0.042
  97. BD (   1) C  41 - C  42        /787. RY*(   2) C  41                  1.04    1.19
0.034
  97. BD (   1) C  41 - C  42        /788. RY*(   3) C  41                  9.87    1.87
0.129
  97. BD (   1) C  41 - C  42        /789. RY*(   4) C  41                  4.89    2.01
0.094
  97. BD (   1) C  41 - C  42        /790. RY*(   5) C  41                  0.94    2.14
0.043
  97. BD (   1) C  41 - C  42        /792. RY*(   7) C  41                  1.58    2.00
0.053
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97. BD (1) C 41 - C 42 /793. RY*(8) C 41 0.69 2.01
0.035
97. BD (1) C 41 - C 42 /794. RY*(9) C 41 18.48 2.21
0.192
97. BD (1) C 41 - C 42 /800. RY*(2) C 42 0.98 1.46
0.036
97. BD (1) C 41 - C 42 /802. RY*(4) C 42 0.97 1.42
0.035
97. BD (1) C 41 - C 42 /805. RY*(7) C 42 0.81 2.25
0.041
97. BD (1) C 41 - C 42 /809. RY*(11) C 42 1.12 2.73
0.053
97. BD (1) C 41 - C 42 /814. RY*(2) C 43 0.54 1.15
0.024
97. BD (1) C 41 - C 42 /815. RY*(3) C 43 0.75 1.30
0.030
97. BD (1) C 41 - C 42 /816. RY*(4) C 43 0.97 1.72
0.039
97. BD (1) C 41 - C 42 /855. RY*(1) C 46 1.07 1.80
0.042
97. BD (1) C 41 - C 42 /861. RY*(7) C 46 1.10 2.18
0.047
97. BD (1) C 41 - C 42 /865. RY*(11) C 46 0.95 2.86
0.050
97. BD (1) C 41 - C 42 /867. RY*(13) C 46 0.78 2.85
0.045
97. BD (1) C 41 - C 42 /***. BD*(1) C 10 - N 11 1.61 0.75
0.033
97. BD (1) C 41 - C 42 /***. BD*(1) N 11 - C 12 1.43 0.75
0.031
97. BD (1) C 41 - C 42 /***. BD*(2) N 11 - C 41 257.93 1.40
0.568
97. BD (1) C 41 - C 42 /***. BD*(1) C 41 - C 42 19.91 1.04
0.136
97. BD (1) C 41 - C 42 /***. BD*(1) C 41 - C 46 30.24 1.05
0.168
97. BD (1) C 41 - C 42 /***. BD*(2) C 41 - C 46 11.43 0.43
0.065
97. BD (1) C 41 - C 42 /***. BD*(1) C 42 - C 47 0.76 0.74
0.022
97. BD (1) C 41 - C 42 /***. BD*(1) C 43 - H 75 3.84 0.76
0.051
97. BD (1) C 41 - C 42 /***. BD*(1) C 45 - C 46 0.88 0.88
0.026
97. BD (1) C 41 - C 42 /***. BD*(1) C 46 - C 49 3.54 0.73
0.048
97. BD (1) C 41 - C 42 /***. BD*(1) C 47 - C 57 1.52 0.71
0.031
98. BD (1) C 41 - C 46 /787. RY*(2) C 41 1.21 1.18
0.036
98. BD (1) C 41 - C 46 /788. RY*(3) C 41 10.73 1.86
0.135
98. BD (1) C 41 - C 46 /789. RY*(4) C 41 4.39 2.00
0.089
98. BD (1) C 41 - C 46 /790. RY*(5) C 41 0.63 2.13
0.035
98. BD (1) C 41 - C 46 /792. RY*(7) C 41 1.94 1.98
0.059
98. BD (1) C 41 - C 46 /793. RY*(8) C 41 0.69 2.00
0.035
98. BD (1) C 41 - C 46 /794. RY*(9) C 41 19.22 2.19
0.196
98. BD (1) C 41 - C 46 /799. RY*(1) C 42 0.60 1.76
0.031
98. BD (1) C 41 - C 46 /805. RY*(7) C 42 1.51 2.24
0.056
98. BD (1) C 41 - C 46 /809. RY*(11) C 42 0.79 2.72
0.044
98. BD (1) C 41 - C 46 /811. RY*(13) C 42 0.57 2.79
0.038

98. BD (1) C 41 - C 46 /842. RY*(2) C 45 1.57 1.50
0.046
98. BD (1) C 41 - C 46 /844. RY*(4) C 45 1.04 1.71
0.040
98. BD (1) C 41 - C 46 /855. RY*(1) C 46 1.04 1.79
0.041
98. BD (1) C 41 - C 46 /856. RY*(2) C 46 1.01 1.53
0.038
98. BD (1) C 41 - C 46 /858. RY*(4) C 46 1.65 1.39
0.046
98. BD (1) C 41 - C 46 /865. RY*(11) C 46 1.09 2.84
0.053
98. BD (1) C 41 - C 46 /867. RY*(13) C 46 0.63 2.84
0.040
98. BD (1) C 41 - C 46 /898. RY*(2) C 49 0.71 1.90
0.035
98. BD (1) C 41 - C 46 /902. RY*(6) C 49 0.52 1.58
0.027
98. BD (1) C 41 - C 46 /***. BD*(1) C 10 - N 11 1.99 0.74
0.036
98. BD (1) C 41 - C 46 /***. BD*(1) N 11 - C 12 0.71 0.73
0.022
98. BD (1) C 41 - C 46 /***. BD*(1) N 11 - C 41 1.54 0.70
0.031
98. BD (1) C 41 - C 46 /***. BD*(2) N 11 - C 41 285.62 1.39
0.593
98. BD (1) C 41 - C 46 /***. BD*(1) C 41 - C 42 32.29 1.03
0.173
98. BD (1) C 41 - C 46 /***. BD*(1) C 41 - C 46 21.41 1.03
0.141
98. BD (1) C 41 - C 46 /***. BD*(2) C 41 - C 46 11.68 0.42
0.064
98. BD (1) C 41 - C 46 /***. BD*(1) C 42 - C 43 0.72 0.87
0.024
98. BD (1) C 41 - C 46 /***. BD*(1) C 42 - C 47 3.14 0.73
0.045
98. BD (1) C 41 - C 46 /***. BD*(1) C 45 - H 73 4.03 0.74
0.052
98. BD (1) C 41 - C 46 /***. BD*(1) C 46 - C 49 0.72 0.72
0.022
98. BD (1) C 41 - C 46 /***. BD*(1) C 49 - C 50 0.86 0.68
0.023
98. BD (1) C 41 - C 46 /***. BD*(1) C 49 - C 58 0.99 0.68
0.025
99. BD (2) C 41 - C 46 /788. RY*(3) C 41 1.20 1.67
0.044
99. BD (2) C 41 - C 46 /789. RY*(4) C 41 0.53 1.81
0.030
99. BD (2) C 41 - C 46 /794. RY*(9) C 41 2.64 2.00
0.071
99. BD (2) C 41 - C 46 /843. RY*(3) C 45 1.44 0.73
0.032
99. BD (2) C 41 - C 46 /***. BD*(1) C 10 - N 11 3.32 0.55
0.041
99. BD (2) C 41 - C 46 /***. BD*(1) N 11 - C 12 2.92 0.54
0.039
99. BD (2) C 41 - C 46 /***. BD*(2) N 11 - C 41 25.32 1.20
0.160
99. BD (2) C 41 - C 46 /***. BD*(1) C 41 - C 42 5.32 0.84
0.065
99. BD (2) C 41 - C 46 /***. BD*(1) C 41 - C 46 5.13 0.84
0.064
99. BD (2) C 41 - C 46 /***. BD*(2) C 41 - C 46 2.35 0.23
0.021
99. BD (2) C 41 - C 46 /***. BD*(2) C 42 - C 43 16.81 0.22
0.054
99. BD (2) C 41 - C 46 /***. BD*(2) C 44 - C 45 15.06 0.21
0.050
99. BD (2) C 41 - C 46 /***. BD*(1) C 49 - C 50 2.47 0.49
0.034

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  99. BD (   2) C  41 - C  46        /***. BD*(   1) C  49 - C  58           2.14    0.49
0.032
 100. BD (   1) C  42 - C  43        /786. RY*(   1) C  41                  0.83    1.92
0.036
 100. BD (   1) C  42 - C  43        /828. RY*(   2) C  44                  0.93    1.82
0.037
 100. BD (   1) C  42 - C  43        /869. RY*(   1) C  47                  0.56    1.68
0.028
 100. BD (   1) C  42 - C  43        /***. BD*(   1) N  11 - C  41          5.04    0.93
0.061
 100. BD (   1) C  42 - C  43        /***. BD*(   2) N  11 - C  41          1.13    1.62
0.043
 100. BD (   1) C  42 - C  43        /***. BD*(   1) C  41 - C  42          1.45    1.26
0.038
 100. BD (   1) C  42 - C  43        /***. BD*(   1) C  42 - C  47          0.70    0.96
0.023
 100. BD (   1) C  42 - C  43        /***. BD*(   1) C  43 - C  44          1.58    1.12
0.038
 100. BD (   1) C  42 - C  43        /***. BD*(   1) C  44 - H  74          2.53    0.97
0.044
 100. BD (   1) C  42 - C  43        /***. BD*(   1) C  47 - H  80          0.81    0.98
0.025
 101. BD (   2) C  42 - C  43        /829. RY*(   3) C  44                  0.83    0.79
0.025
 101. BD (   2) C  42 - C  43        /***. BD*(   2) C  41 - C  46         12.82    0.24
0.050
 101. BD (   2) C  42 - C  43        /***. BD*(   2) C  44 - C  45         16.59    0.22
0.054
 101. BD (   2) C  42 - C  43        /***. BD*(   1) C  47 - C  48          2.59    0.51
0.036
 101. BD (   2) C  42 - C  43        /***. BD*(   1) C  47 - C  57          0.58    0.52
0.017
 101. BD (   2) C  42 - C  43        /***. BD*(   1) C  47 - H  80          0.77    0.57
0.021
 102. BD (   1) C  42 - C  47        /786. RY*(   1) C  41                  1.48    1.84
0.047
 102. BD (   1) C  42 - C  47        /813. RY*(   1) C  43                  0.86    1.97
0.037
 102. BD (   1) C  42 - C  47        /***. BD*(   2) N  11 - C  41          3.55    1.54
0.074
 102. BD (   1) C  42 - C  47        /***. BD*(   1) C  41 - C  46          1.79    1.18
0.041
 102. BD (   1) C  42 - C  47        /***. BD*(   1) C  42 - C  43          0.76    1.02
0.025
 102. BD (   1) C  42 - C  47        /***. BD*(   1) C  43 - C  44          2.84    1.03
0.048
 102. BD (   1) C  42 - C  47        /***. BD*(   1) C  48 - H 126          1.43    0.88
0.032
 102. BD (   1) C  42 - C  47        /***. BD*(   1) C  57 - H 123          1.15    0.89
0.029
 103. BD (   1) C  43 - C  44        /799. RY*(   1) C  42                  1.24    2.00
0.045
 103. BD (   1) C  43 - C  44        /842. RY*(   2) C  45                  0.65    1.74
0.030
 103. BD (   1) C  43 - C  44        /***. BD*(   1) C  42 - C  43          1.78    1.11
0.040
 103. BD (   1) C  43 - C  44        /***. BD*(   1) C  42 - C  47          3.95    0.97
0.055
 103. BD (   1) C  43 - C  44        /***. BD*(   1) C  44 - C  45          1.52    1.12
0.037
 103. BD (   1) C  43 - C  44        /***. BD*(   1) C  45 - H  73          2.72    0.98
0.046
 104. BD (   1) C  43 - H  75        /799. RY*(   1) C  42                  1.62    1.82
0.049
 104. BD (   1) C  43 - H  75        /827. RY*(   1) C  44                  0.98    1.64
0.036
 104. BD (   1) C  43 - H  75        /***. BD*(   1) C  41 - C  42          3.67    1.09
0.056
 104. BD (   1) C  43 - H  75        /***. BD*(   1) C  44 - C  45          3.98    0.94
0.055
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105. BD (1) C 44 - C 45   /813. RY*(1) C 43   0.52   2.06
0.029
105. BD (1) C 44 - C 45   /855. RY*(1) C 46   1.39   2.03
0.048
105. BD (1) C 44 - C 45   /***. BD*(1) C 43 - C 44   1.48   1.13
0.036
105. BD (1) C 44 - C 45   /***. BD*(1) C 43 - H 75   2.55   0.99
0.045
105. BD (1) C 44 - C 45   /***. BD*(1) C 45 - C 46   1.83   1.11
0.040
105. BD (1) C 44 - C 45   /***. BD*(1) C 46 - C 49   4.03   0.96
0.056
106. BD (2) C 44 - C 45   /***. BD*(2) C 41 - C 46   14.95   0.25
0.055
106. BD (2) C 44 - C 45   /***. BD*(2) C 42 - C 43   13.20   0.24
0.050
107. BD (1) C 44 - H 74   /813. RY*(1) C 43   1.42   1.88
0.046
107. BD (1) C 44 - H 74   /841. RY*(1) C 45   1.43   1.87
0.046
107. BD (1) C 44 - H 74   /***. RY*(1) H 73   0.52   1.07
0.021
107. BD (1) C 44 - H 74   /***. RY*(1) H 75   0.52   1.07
0.021
107. BD (1) C 44 - H 74   /***. BD*(1) C 42 - C 43   4.53   0.93
0.058
107. BD (1) C 44 - H 74   /***. BD*(1) C 45 - C 46   4.55   0.93
0.058
108. BD (1) C 45 - C 46   /786. RY*(1) C 41   0.83   1.92
0.036
108. BD (1) C 45 - C 46   /828. RY*(2) C 44   0.95   1.82
0.037
108. BD (1) C 45 - C 46   /897. RY*(1) C 49   0.76   1.74
0.033
108. BD (1) C 45 - C 46   /***. BD*(1) N 11 - C 41   4.96   0.94
0.061
108. BD (1) C 45 - C 46   /***. BD*(2) N 11 - C 41   0.80   1.63
0.036
108. BD (1) C 45 - C 46   /***. BD*(1) C 41 - C 46   1.83   1.27
0.043
108. BD (1) C 45 - C 46   /***. BD*(1) C 44 - C 45   1.60   1.12
0.038
108. BD (1) C 45 - C 46   /***. BD*(1) C 44 - H 74   2.59   0.97
0.045
108. BD (1) C 45 - C 46   /***. BD*(1) C 46 - C 49   0.69   0.95
0.023
108. BD (1) C 45 - C 46   /***. BD*(1) C 49 - H 79   1.06   0.95
0.028
109. BD (1) C 45 - H 73   /827. RY*(1) C 44   1.00   1.65
0.036
109. BD (1) C 45 - H 73   /855. RY*(1) C 46   1.66   1.85
0.050
109. BD (1) C 45 - H 73   /***. BD*(1) C 41 - C 46   3.56   1.10
0.056
109. BD (1) C 45 - H 73   /***. BD*(1) C 43 - C 44   3.90   0.94
0.054
110. BD (1) C 46 - C 49   /786. RY*(1) C 41   1.51   1.84
0.047
110. BD (1) C 46 - C 49   /841. RY*(1) C 45   0.91   1.97
0.038
110. BD (1) C 46 - C 49   /***. BD*(2) N 11 - C 41   3.66   1.55
0.076
110. BD (1) C 46 - C 49   /***. BD*(1) C 41 - C 42   1.72   1.19
0.040
110. BD (1) C 46 - C 49   /***. BD*(1) C 44 - C 45   2.79   1.04
0.048
110. BD (1) C 46 - C 49   /***. BD*(1) C 45 - C 46   0.74   1.02
0.025
110. BD (1) C 46 - C 49   /***. BD*(1) C 50 - H 129   1.43   0.87
0.032

110. BD (1) C 46 - C 49	/***. BD*(1) C 58 - H 132	1.41	0.87	0.032
111. BD (1) C 47 - C 48	/801. RY*(3) C 42	0.74	1.35	0.028
111. BD (1) C 47 - C 48	/***. RY*(1) C 57	0.55	1.30	0.024
111. BD (1) C 47 - C 48	/***. BD*(1) C 41 - C 42	0.66	1.16	0.025
111. BD (1) C 47 - C 48	/***. BD*(1) C 42 - C 43	0.84	0.99	0.026
111. BD (1) C 47 - C 48	/***. BD*(2) C 42 - C 43	2.95	0.53	0.038
111. BD (1) C 47 - C 48	/***. BD*(1) C 57 - H 125	1.69	0.87	0.034
112. BD (1) C 47 - C 57	/800. RY*(2) C 42	0.69	1.57	0.030
112. BD (1) C 47 - C 57	/***. BD*(1) C 41 - C 42	2.74	1.16	0.050
112. BD (1) C 47 - C 57	/***. BD*(2) C 42 - C 43	0.56	0.53	0.017
112. BD (1) C 47 - C 57	/***. BD*(1) C 42 - C 47	0.59	0.86	0.020
112. BD (1) C 47 - C 57	/***. BD*(1) C 48 - H 127	1.70	0.86	0.034
113. BD (1) C 47 - H 80	/***. BD*(1) C 42 - C 43	4.35	0.88	0.055
113. BD (1) C 47 - H 80	/***. BD*(2) C 42 - C 43	1.03	0.41	0.020
113. BD (1) C 47 - H 80	/***. BD*(1) C 48 - H 128	2.74	0.73	0.040
113. BD (1) C 47 - H 80	/***. BD*(1) C 57 - H 124	2.98	0.73	0.042
114. BD (1) C 48 - H 126	/***. BD*(1) C 42 - C 47	3.29	0.76	0.045
115. BD (1) C 48 - H 127	/***. BD*(1) C 47 - C 57	2.88	0.74	0.041
116. BD (1) C 48 - H 128	/***. BD*(1) C 47 - H 80	2.16	0.78	0.037
117. BD (1) C 49 - C 50	/857. RY*(3) C 46	0.81	1.27	0.029
117. BD (1) C 49 - C 50	/***. BD*(1) C 41 - C 46	1.62	1.17	0.039
117. BD (1) C 49 - C 50	/***. BD*(2) C 41 - C 46	1.97	0.56	0.033
117. BD (1) C 49 - C 50	/***. BD*(1) C 46 - C 49	0.54	0.86	0.019
117. BD (1) C 49 - C 50	/***. BD*(1) C 58 - H 133	1.57	0.88	0.033
118. BD (1) C 49 - C 58	/***. BD*(1) C 41 - C 46	1.81	1.17	0.041
118. BD (1) C 49 - C 58	/***. BD*(2) C 41 - C 46	1.89	0.56	0.032
118. BD (1) C 49 - C 58	/***. BD*(1) C 46 - C 49	0.59	0.86	0.020
118. BD (1) C 49 - C 58	/***. BD*(1) C 50 - H 131	1.64	0.86	0.034
119. BD (1) C 49 - H 79	/***. BD*(1) C 45 - C 46	4.84	0.89	0.059
119. BD (1) C 49 - H 79	/***. BD*(1) C 50 - H 130	2.77	0.74	0.041
119. BD (1) C 49 - H 79	/***. BD*(1) C 58 - H 134	2.85	0.74	0.041
120. BD (1) C 50 - H 129	/***. BD*(1) C 46 - C 49	3.33	0.76	0.045
121. BD (1) C 50 - H 130	/***. BD*(1) C 49 - H 79	2.25	0.76	0.037
122. BD (1) C 50 - H 131	/***. BD*(1) C 49 - C 58	3.10	0.73	0.042
123. BD (1) C 51 - C 52	/283. RY*(2) C 5	0.72	1.50	0.030

123. BD (1) C 51 - C 52   /***. BD*(1) C   4 - C   5   2.27   0.99
0.043
123. BD (1) C 51 - C 52   /***. BD*(2) C   4 - C   5   2.17   0.54
0.034
123. BD (1) C 51 - C 52   /***. BD*(1) C   5 - C 51   0.54   0.86
0.019
123. BD (1) C 51 - C 52   /***. BD*(1) C 59 - H 113   1.58   0.88
0.033
124. BD (1) C 51 - C 59   /284. RY*(3) C   5   0.66   1.43
0.028
124. BD (1) C 51 - C 59   /***. BD*(1) C   4 - C   5   2.17   0.99
0.042
124. BD (1) C 51 - C 59   /***. BD*(2) C   4 - C   5   1.82   0.54
0.031
124. BD (1) C 51 - C 59   /***. BD*(1) C   5 - C 51   0.56   0.86
0.020
124. BD (1) C 51 - C 59   /***. BD*(1) C 52 - H 115   1.64   0.86
0.034
125. BD (1) C 51 - H 81   /***. BD*(1) C   5 - C   6   4.79   0.89
0.059
125. BD (1) C 51 - H 81   /***. BD*(1) C 52 - H 116   2.80   0.74
0.041
125. BD (1) C 51 - H 81   /***. BD*(1) C 59 - H 112   2.86   0.74
0.041
126. BD (1) C 52 - H 114   /***. BD*(1) C   5 - C 51   3.34   0.76
0.045
127. BD (1) C 52 - H 115   /***. BD*(1) C 51 - C 59   3.10   0.73
0.042
128. BD (1) C 52 - H 116   /***. BD*(1) C 51 - H 81   2.20   0.76
0.037
129. BD (1) C 53 - C 54   /256. RY*(3) C   3   0.83   1.31
0.030
129. BD (1) C 53 - C 54   /***. BD*(1) C   3 - C   4   0.99   0.98
0.028
129. BD (1) C 53 - C 54   /***. BD*(1) C   3 - C   8   0.75   1.00
0.024
129. BD (1) C 53 - C 54   /***. BD*(2) C   3 - C   8   3.10   0.53
0.039
129. BD (1) C 53 - C 54   /***. BD*(1) C 60 - H 121   1.64   0.88
0.034
130. BD (1) C 53 - C 60   /255. RY*(2) C   3   0.60   1.61
0.028
130. BD (1) C 53 - C 60   /***. BD*(1) C   3 - C   4   3.35   0.98
0.051
130. BD (1) C 53 - C 60   /***. BD*(2) C   3 - C   8   0.61   0.53
0.017
130. BD (1) C 53 - C 60   /***. BD*(1) C   3 - C 53   0.58   0.86
0.020
130. BD (1) C 53 - C 60   /***. BD*(1) C 54 - H 119   1.70   0.86
0.034
131. BD (1) C 53 - H 82   /***. BD*(1) C   3 - C   8   4.57   0.88
0.057
131. BD (1) C 53 - H 82   /***. BD*(2) C   3 - C   8   0.73   0.41
0.017
131. BD (1) C 53 - H 82   /***. BD*(1) C 54 - H 118   2.77   0.73
0.040
131. BD (1) C 53 - H 82   /***. BD*(1) C 60 - H 122   3.02   0.73
0.042
132. BD (1) C 54 - H 117   /***. BD*(1) C   3 - C 53   3.24   0.76
0.045
133. BD (1) C 54 - H 118   /***. BD*(1) C 53 - H 82   2.18   0.78
0.037
134. BD (1) C 54 - H 119   /***. BD*(1) C 53 - C 60   2.89   0.74
0.041
135. BD (1) C 55 - H 108   /***. BD*(1) C 32 - C 37   3.43   0.75
0.045
136. BD (1) C 55 - H 109   /***. BD*(1) C 37 - H 85   2.31   0.75
0.037
137. BD (1) C 55 - H 110   /***. BD*(1) C 37 - C 38   3.25   0.71
0.043

138. BD (1) C 56 - H 102	/***. BD*(1) C 36 - C 39	3.52	0.75	0.046
139. BD (1) C 56 - H 103	/***. BD*(1) C 39 - C 40	3.30	0.71	0.043
140. BD (1) C 56 - H 104	/***. BD*(1) C 39 - H 86	2.23	0.75	0.036
141. BD (1) C 57 - H 123	/***. BD*(1) C 42 - C 47	3.78	0.75	0.048
142. BD (1) C 57 - H 124	/***. BD*(1) C 47 - H 80	1.97	0.78	0.035
143. BD (1) C 57 - H 125	/***. BD*(1) C 47 - C 48	3.13	0.71	0.042
144. BD (1) C 58 - H 132	/***. BD*(1) C 46 - C 49	3.44	0.76	0.046
145. BD (1) C 58 - H 133	/***. BD*(1) C 49 - C 50	3.21	0.72	0.043
146. BD (1) C 58 - H 134	/***. BD*(1) C 49 - H 79	2.23	0.76	0.037
147. BD (1) C 59 - H 111	/***. BD*(1) C 5 - C 51	3.53	0.76	0.046
148. BD (1) C 59 - H 112	/***. BD*(1) C 51 - H 81	2.24	0.76	0.037
149. BD (1) C 59 - H 113	/***. BD*(1) C 51 - C 52	3.22	0.72	0.043
150. BD (1) C 60 - H 120	/***. BD*(1) C 3 - C 53	3.92	0.75	0.049
151. BD (1) C 60 - H 121	/***. BD*(1) C 53 - C 54	3.21	0.71	0.043
152. BD (1) C 60 - H 122	/***. BD*(1) C 53 - H 82	2.04	0.77	0.036
153. BD (1) C 61 - H 96	/***. BD*(1) C 26 - C 29	3.47	0.76	0.046
154. BD (1) C 61 - H 97	/***. BD*(1) C 29 - C 30	3.24	0.71	0.043
155. BD (1) C 61 - H 98	/***. BD*(1) C 29 - H 83	2.28	0.75	0.037
156. BD (1) C 62 - H 87	/***. BD*(1) C 22 - C 27	3.74	0.75	0.048
157. BD (1) C 62 - H 88	/***. BD*(1) C 27 - H 84	2.19	0.75	0.036
158. BD (1) C 62 - H 89	/***. BD*(1) C 27 - C 28	3.25	0.70	0.043
159. CR (1) C 1	/243. RY*(4) O 2	0.75	10.46	0.079
159. CR (1) C 1	/***. BD*(1) C 1 - O 2	0.91	10.26	0.087
159. CR (1) C 1	/***. BD*(1) C 1 - B 14	0.83	10.08	0.084
159. CR (1) C 1	/***. BD*(1) C 1 - B 15	1.91	10.20	0.127
159. CR (1) C 1	/***. BD*(1) C 10 - B 14	0.52	10.18	0.065
159. CR (1) C 1	/***. BD*(1) B 15 - C 16	1.96	10.15	0.128
160. CR (1) O 2	/226. RY*(1) C 1	5.15	19.43	0.284
160. CR (1) O 2	/***. BD*(1) C 1 - B 14	0.87	18.75	0.117
160. CR (1) O 2	/***. BD*(1) C 1 - B 15	1.06	18.87	0.128
161. CR (1) C 3	/270. RY*(3) C 4	1.03	10.87	0.095
161. CR (1) C 3	/325. RY*(2) C 8	1.04	10.72	0.094
161. CR (1) C 3	/***. BD*(1) C 4 - C 5	0.86	10.19	0.084
161. CR (1) C 3	/***. BD*(1) C 4 - N 9	0.84	10.04	0.083
161. CR (1) C 3	/***. BD*(1) C 7 - C 8	0.58	10.22	0.069

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 162. CR (   1) C   4              /254. RY*(   1) C   3                  0.80   11.13
0.084
 162. CR (   1) C   4              /255. RY*(   2) C   3                  0.68   10.86
0.077
 162. CR (   1) C   4              /282. RY*(   1) C   5                  0.93   11.18
0.091
 162. CR (   1) C   4              /***. BD*(   1) C   3 - C   4          0.51   10.23
0.065
 162. CR (   1) C   4              /***. BD*(   1) C   3 - C  53          0.74   10.11
0.078
 162. CR (   1) C   4              /***. BD*(   1) C   4 - C   5          0.50   10.23
0.065
 162. CR (   1) C   4              /***. BD*(   1) C   4 - N   9          0.68   10.08
0.075
 162. CR (   1) C   4              /***. BD*(   1) C   5 - C   6          0.50   10.24
0.064
 162. CR (   1) C   4              /***. BD*(   1) C   5 - C  51          0.80   10.10
0.081
 162. CR (   1) C   4              /***. BD*(   1) N   9 - C  10          0.97   10.12
0.089
 162. CR (   1) C   4              /***. BD*(   1) N   9 - C  13          0.72   10.12
0.077
 163. CR (   1) C   5              /270. RY*(   3) C   4                  1.11   10.88
0.098
 163. CR (   1) C   5              /297. RY*(   2) C   6                  1.34   10.85
0.108
 163. CR (   1) C   5              /926. RY*(   2) C  51                  0.77   11.25
0.083
 163. CR (   1) C   5              /***. BD*(   1) C   3 - C   4          0.84   10.20
0.083
 163. CR (   1) C   5              /***. BD*(   1) C   4 - N   9          0.84   10.05
0.083
 163. CR (   1) C   5              /***. BD*(   1) C   6 - C   7          0.55   10.23
0.067
 164. CR (   1) C   6              /283. RY*(   2) C   5                  1.03   10.69
0.094
 164. CR (   1) C   6              /284. RY*(   3) C   5                  0.89   10.62
0.087
 164. CR (   1) C   6              /311. RY*(   2) C   7                  1.54   10.93
0.116
 164. CR (   1) C   6              /***. RY*(   2) H  78                  0.50   11.96
0.069
 164. CR (   1) C   6              /***. BD*(   1) C   4 - C   5          0.55   10.19
0.067
 164. CR (   1) C   6              /***. BD*(   1) C   5 - C  51          0.74   10.05
0.077
 164. CR (   1) C   6              /***. BD*(   1) C   7 - C   8          0.55   10.22
0.067
 165. CR (   1) C   7              /297. RY*(   2) C   6                  1.20   10.84
0.102
 165. CR (   1) C   7              /325. RY*(   2) C   8                  0.93   10.72
0.089
 165. CR (   1) C   7              /***. BD*(   1) C   3 - C   8          0.65   10.21
0.073
 165. CR (   1) C   7              /***. BD*(   1) C   5 - C   6          0.64   10.20
0.073
 166. CR (   1) C   8              /255. RY*(   2) C   3                  1.68   10.81
0.121
 166. CR (   1) C   8              /311. RY*(   2) C   7                  1.43   10.93
0.111
 166. CR (   1) C   8              /***. BD*(   1) C   3 - C   4          0.54   10.18
0.067
 166. CR (   1) C   8              /***. BD*(   1) C   3 - C  53          0.76   10.06
0.078
 166. CR (   1) C   8              /***. BD*(   1) C   6 - C   7          0.56   10.21
0.068
 167. CR (   1) N   9              /268. RY*(   1) C   4                  0.78   15.21
0.097
 167. CR (   1) N   9              /396. RY*(   3) C  13                  0.94   14.91
0.106
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 167. CR (   1) N   9              /***. BD*(   1) C  10 - B  14           0.65   14.29
0.086
 168. CR (   1) C  10              /408. RY*(   1) B  14                  1.11   11.31
0.100
 168. CR (   1) C  10              /411. RY*(   4) B  14                  0.74   11.01
0.081
 168. CR (   1) C  10              /***. BD*(   1) C   4 - N   9          1.23   10.10
0.100
 168. CR (   1) C  10              /***. BD*(   1) N   9 - C  13          0.53   10.14
0.066
 168. CR (   1) C  10              /***. BD*(   1) C  10 - B  14          1.85   10.23
0.124
 168. CR (   1) C  10              /***. BD*(   1) N  11 - C  12          0.52   10.13
0.065
 168. CR (   1) C  10              /***. BD*(   1) N  11 - C  41          1.29   10.10
0.103
 168. CR (   1) C  10              /***. BD*(   1) B  14 - B  15          1.98   10.28
0.129
 169. CR (   1) N  11              /354. RY*(   3) C  10                  0.93   15.53
0.107
 169. CR (   1) N  11              /382. RY*(   3) C  12                  0.81   14.93
0.098
 169. CR (   1) N  11              /786. RY*(   1) C  41                  0.71   15.15
0.093
 169. CR (   1) N  11              /***. BD*(   1) C  10 - B  14          0.69   14.29
0.089
 170. CR (   1) C  12              /368. RY*(   3) N  11                  0.72   10.86
0.079
 170. CR (   1) C  12              /395. RY*(   2) C  13                  1.07   11.10
0.097
 170. CR (   1) C  12              /396. RY*(   3) C  13                  0.98   10.84
0.092
 170. CR (   1) C  12              /***. RY*(   1) H  71                  0.57   11.57
0.073
 170. CR (   1) C  12              /***. BD*(   1) C  10 - N  11          0.69   10.12
0.075
 170. CR (   1) C  12              /***. BD*(   1) N  11 - C  41          1.11   10.08
0.095
 170. CR (   1) C  12              /***. BD*(   1) C  12 - C  13          1.15   10.28
0.097
 170. CR (   1) C  12              /***. BD*(   1) C  13 - H  72          1.05   10.11
0.092
 171. CR (   1) C  13              /340. RY*(   3) N   9                  0.74   10.84
0.080
 171. CR (   1) C  13              /381. RY*(   2) C  12                  1.05   11.11
0.096
 171. CR (   1) C  13              /382. RY*(   3) C  12                  1.08   10.84
0.097
 171. CR (   1) C  13              /***. RY*(   1) H  72                  0.56   11.54
0.072
 171. CR (   1) C  13              /***. BD*(   1) C   4 - N   9          1.14   10.08
0.097
 171. CR (   1) C  13              /***. BD*(   1) N   9 - C  10          0.68   10.12
0.075
 171. CR (   1) C  13              /***. BD*(   1) C  12 - C  13          1.15   10.28
0.097
 171. CR (   1) C  13              /***. BD*(   1) C  12 - H  71          1.05   10.11
0.092
 172. CR (   1) B  14              /352. RY*(   1) C  10                  0.77    7.97
0.070
 172. CR (   1) B  14              /422. RY*(   1) B  15                  1.28    7.95
0.090
 172. CR (   1) B  14              /***. BD*(   1) C   1 - O   2          1.80    6.84
0.100
 172. CR (   1) B  14              /***. BD*(   1) C   1 - B  14          0.95    6.66
0.073
 172. CR (   1) B  14              /***. BD*(   1) C   1 - B  15          1.43    6.77
0.089
 172. CR (   1) B  14              /***. BD*(   1) N   9 - C  10          1.39    6.67
0.087
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 172. CR (   1) B  14              /***. BD*(   1) C  10 - N  11           1.54    6.67
0.091
 172. CR (   1) B  14              /***. BD*(   1) B  14 - B  15           1.20    6.81
0.081
 172. CR (   1) B  14              /***. BD*(   1) B  15 - C  16           4.41    6.73
0.156
 173. CR (   1) B  15              /226. RY*(   1) C   1                   1.19    7.33
0.084
 173. CR (   1) B  15              /408. RY*(   1) B  14                   1.65    7.83
0.102
 173. CR (   1) B  15              /436. RY*(   1) C  16                   0.90    8.13
0.077
 173. CR (   1) B  15              /***. BD*(   1) C   1 - O   2           4.53    6.83
0.159
 173. CR (   1) B  15              /***. BD*(   1) C   1 - B  14           1.25    6.65
0.084
 173. CR (   1) B  15              /***. BD*(   1) C   1 - B  15           0.80    6.76
0.067
 173. CR (   1) B  15              /***. BD*(   1) C  10 - B  14           4.41    6.75
0.155
 173. CR (   1) B  15              /***. BD*(   1) B  14 - B  15           1.28    6.80
0.084
 173. CR (   1) B  15              /***. BD*(   1) C  16 - N  17           1.24    6.67
0.082
 173. CR (   1) B  15              /***. BD*(   1) C  16 - N  20           1.67    6.67
0.095
 174. CR (   1) C  16              /423. RY*(   2) B  15                   0.64   11.17
0.076
 174. CR (   1) C  16              /452. RY*(   3) N  17                   0.55   10.76
0.068
 174. CR (   1) C  16              /***. BD*(   1) B  14 - B  15           1.35   10.29
0.106
 174. CR (   1) C  16              /***. BD*(   1) B  15 - C  16           1.58   10.22
0.115
 174. CR (   1) C  16              /***. BD*(   1) N  17 - C  18           0.57   10.14
0.068
 174. CR (   1) C  16              /***. BD*(   1) N  17 - C  21           1.31   10.10
0.104
 174. CR (   1) C  16              /***. BD*(   1) C  19 - N  20           0.56   10.14
0.068
 174. CR (   1) C  16              /***. BD*(   1) N  20 - C  31           1.32   10.10
0.104
 175. CR (   1) N  17              /439. RY*(   4) C  16                   1.01   15.39
0.112
 175. CR (   1) N  17              /466. RY*(   3) C  18                   0.97   14.98
0.108
 175. CR (   1) N  17              /506. RY*(   1) C  21                   0.68   15.13
0.091
 175. CR (   1) N  17              /***. BD*(   1) B  15 - C  16           0.60   14.28
0.084
 176. CR (   1) C  18              /452. RY*(   3) N  17                   0.85   10.75
0.085
 176. CR (   1) C  18              /479. RY*(   2) C  19                   1.03   11.08
0.096
 176. CR (   1) C  18              /480. RY*(   3) C  19                   0.96   10.88
0.091
 176. CR (   1) C  18              /***. RY*(   1) H  63                   0.58   11.59
0.073
 176. CR (   1) C  18              /***. BD*(   1) C  16 - N  17           0.74   10.15
0.078
 176. CR (   1) C  18              /***. BD*(   1) N  17 - C  21           1.17   10.08
0.098
 176. CR (   1) C  18              /***. BD*(   1) C  18 - C  19           1.03   10.27
0.092
 176. CR (   1) C  18              /***. BD*(   1) C  19 - H  64           1.01   10.11
0.090
 177. CR (   1) C  19              /465. RY*(   2) C  18                   1.09   11.13
0.098
 177. CR (   1) C  19              /466. RY*(   3) C  18                   0.91   10.91
0.089
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177. CR (1) C 19 /494. RY*(3) N 20 0.80 10.83
0.083
177. CR (1) C 19 /***. RY*(1) H 64 0.56 11.56
0.072
177. CR (1) C 19 /***. BD*(1) C 16 - N 20 0.73 10.15
0.078
177. CR (1) C 19 /***. BD*(1) C 18 - C 19 1.04 10.27
0.093
177. CR (1) C 19 /***. BD*(1) C 18 - H 63 1.00 10.11
0.090
177. CR (1) C 19 /***. BD*(1) N 20 - C 31 1.12 10.08
0.096
178. CR (1) N 20 /480. RY*(3) C 19 0.90 14.96
0.104
178. CR (1) N 20 /646. RY*(1) C 31 0.71 15.18
0.093
178. CR (1) N 20 /***. BD*(1) B 15 - C 16 0.63 14.28
0.086
179. CR (1) C 21 /520. RY*(1) C 22 0.82 11.07
0.085
179. CR (1) C 21 /522. RY*(3) C 22 0.51 10.75
0.066
179. CR (1) C 21 /576. RY*(1) C 26 0.99 11.18
0.094
179. CR (1) C 21 /***. BD*(1) C 16 - N 17 1.03 10.13
0.092
179. CR (1) C 21 /***. BD*(1) N 17 - C 18 0.69 10.11
0.075
179. CR (1) C 21 /***. BD*(1) N 17 - C 21 0.79 10.07
0.080
179. CR (1) C 21 /***. BD*(1) C 21 - C 22 0.53 10.23
0.067
179. CR (1) C 21 /***. BD*(1) C 21 - C 26 0.54 10.23
0.067
179. CR (1) C 21 /***. BD*(1) C 22 - C 27 0.77 10.11
0.079
179. CR (1) C 21 /***. BD*(1) C 26 - C 29 0.83 10.10
0.082
180. CR (1) C 22 /508. RY*(3) C 21 0.91 10.72
0.088
180. CR (1) C 22 /535. RY*(2) C 23 0.82 10.59
0.083
180. CR (1) C 22 /536. RY*(3) C 23 0.61 10.58
0.072
180. CR (1) C 22 /592. RY*(3) C 27 0.50 11.24
0.067
180. CR (1) C 22 /***. BD*(1) N 17 - C 21 0.88 10.03
0.085
180. CR (1) C 22 /***. BD*(1) C 21 - C 26 0.88 10.19
0.085
180. CR (1) C 22 /***. BD*(1) C 23 - C 24 0.57 10.23
0.068
181. CR (1) C 23 /522. RY*(3) C 22 1.62 10.69
0.118
181. CR (1) C 23 /549. RY*(2) C 24 1.40 10.93
0.110
181. CR (1) C 23 /***. RY*(2) H 67 0.50 11.95
0.069
181. CR (1) C 23 /***. BD*(1) C 21 - C 22 0.55 10.18
0.068
181. CR (1) C 23 /***. BD*(1) C 22 - C 27 0.78 10.06
0.080
181. CR (1) C 23 /***. BD*(1) C 24 - C 25 0.56 10.21
0.068
182. CR (1) C 24 /535. RY*(2) C 23 0.76 10.58
0.080
182. CR (1) C 24 /563. RY*(2) C 25 1.20 10.83
0.102
182. CR (1) C 24 /***. BD*(1) C 22 - C 23 0.66 10.21
0.074

182. CR (1) C 24 /***. BD*(1) C 25 - C 26 0.64 10.20
0.073
183. CR (1) C 25 /549. RY*(2) C 24 1.56 10.93
0.117
183. CR (1) C 25 /578. RY*(3) C 26 1.54 10.79
0.115
183. CR (1) C 25 /***. BD*(1) C 21 - C 26 0.56 10.18
0.068
183. CR (1) C 25 /***. BD*(1) C 23 - C 24 0.53 10.22
0.066
183. CR (1) C 25 /***. BD*(1) C 26 - C 29 0.75 10.05
0.078
184. CR (1) C 26 /508. RY*(3) C 21 1.09 10.72
0.096
184. CR (1) C 26 /563. RY*(2) C 25 1.33 10.84
0.107
184. CR (1) C 26 /619. RY*(2) C 29 0.76 11.31
0.083
184. CR (1) C 26 /***. BD*(1) N 17 - C 21 0.85 10.03
0.083
184. CR (1) C 26 /***. BD*(1) C 21 - C 22 0.87 10.20
0.085
184. CR (1) C 26 /***. BD*(1) C 24 - C 25 0.55 10.23
0.067
185. CR (1) C 27 /520. RY*(1) C 22 0.92 11.04
0.090
185. CR (1) C 27 /606. RY*(3) C 28 0.67 10.88
0.076
185. CR (1) C 27 /***. RY*(3) C 62 0.68 10.82
0.077
185. CR (1) C 27 /***. BD*(1) C 21 - C 22 0.62 10.20
0.072
185. CR (1) C 27 /***. BD*(1) C 22 - C 23 0.55 10.22
0.067
186. CR (1) C 28 /591. RY*(2) C 27 0.58 10.75
0.071
186. CR (1) C 28 /594. RY*(5) C 27 0.58 11.19
0.072
187. CR (1) C 29 /576. RY*(1) C 26 0.86 11.15
0.087
187. CR (1) C 29 /634. RY*(3) C 30 0.69 10.78
0.077
187. CR (1) C 29 /***. RY*(3) C 61 0.64 10.56
0.074
187. CR (1) C 29 /***. BD*(1) C 21 - C 26 0.65 10.21
0.073
187. CR (1) C 29 /***. BD*(1) C 25 - C 26 0.50 10.22
0.064
188. CR (1) C 30 /620. RY*(3) C 29 0.55 10.77
0.069
188. CR (1) C 30 /***. RY*(2) H 93 0.59 11.53
0.074
189. CR (1) C 31 /660. RY*(1) C 32 0.91 11.19
0.090
189. CR (1) C 31 /716. RY*(1) C 36 0.97 11.17
0.093
189. CR (1) C 31 /***. BD*(1) C 16 - N 20 1.03 10.14
0.092
189. CR (1) C 31 /***. BD*(1) C 19 - N 20 0.67 10.11
0.074
189. CR (1) C 31 /***. BD*(1) N 20 - C 31 0.73 10.07
0.077
189. CR (1) C 31 /***. BD*(1) C 31 - C 32 0.51 10.23
0.065
189. CR (1) C 31 /***. BD*(1) C 31 - C 36 0.54 10.24
0.067
189. CR (1) C 31 /***. BD*(1) C 32 - C 37 0.79 10.10
0.080
189. CR (1) C 31 /***. BD*(1) C 36 - C 39 0.78 10.11
0.080

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 190. CR (   1) C  32              /648. RY*(   3) C  31                   1.11   10.84
0.098
 190. CR (   1) C  32              /675. RY*(   2) C  33                   0.94   10.67
0.090
 190. CR (   1) C  32              /731. RY*(   2) C  37                   0.72   11.30
0.080
 190. CR (   1) C  32              /***. BD*(   1) N  20 - C  31           0.84   10.04
0.083
 190. CR (   1) C  32              /***. BD*(   1) C  31 - C  36           0.86   10.20
0.084
 190. CR (   1) C  32              /***. BD*(   1) C  33 - C  34           0.56   10.23
0.068
 191. CR (   1) C  33              /661. RY*(   2) C  32                   0.94   10.66
0.090
 191. CR (   1) C  33              /662. RY*(   3) C  32                   0.90   10.61
0.087
 191. CR (   1) C  33              /689. RY*(   2) C  34                   1.49   10.93
0.114
 191. CR (   1) C  33              /***. RY*(   2) H  70                   0.51   11.96
0.070
 191. CR (   1) C  33              /***. BD*(   1) C  31 - C  32           0.53   10.18
0.066
 191. CR (   1) C  33              /***. BD*(   1) C  32 - C  37           0.76   10.05
0.079
 191. CR (   1) C  33              /***. BD*(   1) C  34 - C  35           0.56   10.22
0.068
 192. CR (   1) C  34              /675. RY*(   2) C  33                   0.82   10.67
0.083
 192. CR (   1) C  34              /703. RY*(   2) C  35                   1.21   10.82
0.102
 192. CR (   1) C  34              /***. BD*(   1) C  32 - C  33           0.64   10.20
0.072
 192. CR (   1) C  34              /***. BD*(   1) C  35 - C  36           0.64   10.20
0.073
 193. CR (   1) C  35              /689. RY*(   2) C  34                   1.48   10.93
0.114
 193. CR (   1) C  35              /717. RY*(   2) C  36                   1.70   10.85
0.121
 193. CR (   1) C  35              /***. BD*(   1) C  31 - C  36           0.54   10.19
0.067
 193. CR (   1) C  35              /***. BD*(   1) C  33 - C  34           0.55   10.21
0.067
 193. CR (   1) C  35              /***. BD*(   1) C  36 - C  39           0.75   10.06
0.078
 194. CR (   1) C  36              /648. RY*(   3) C  31                   1.07   10.84
0.096
 194. CR (   1) C  36              /703. RY*(   2) C  35                   1.35   10.83
0.108
 194. CR (   1) C  36              /759. RY*(   2) C  39                   0.65   11.31
0.076
 194. CR (   1) C  36              /***. BD*(   1) N  20 - C  31           0.85   10.04
0.083
 194. CR (   1) C  36              /***. BD*(   1) C  31 - C  32           0.87   10.19
0.085
 194. CR (   1) C  36              /***. BD*(   1) C  34 - C  35           0.56   10.23
0.068
 195. CR (   1) C  37              /660. RY*(   1) C  32                   0.86   11.16
0.088
 195. CR (   1) C  37              /746. RY*(   3) C  38                   0.74   10.80
0.080
 195. CR (   1) C  37              /983. RY*(   3) C  55                   0.65   10.67
0.074
 195. CR (   1) C  37              /***. BD*(   1) C  31 - C  32           0.62   10.20
0.071
 195. CR (   1) C  37              /***. BD*(   1) C  32 - C  33           0.53   10.22
0.066
 196. CR (   1) C  38              /***. RY*(   2) H 105                   0.60   11.52
0.074
 197. CR (   1) C  39              /716. RY*(   1) C  36                   0.87   11.14
0.088
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 197. CR (   1) C  39              /774. RY*(   3) C  40                  0.69   10.85
0.077
 197. CR (   1) C  39              /997. RY*(   3) C  56                  0.69   10.60
0.076
 197. CR (   1) C  39              /***. BD*(   1) C  31 - C  36          0.63   10.20
0.072
 197. CR (   1) C  39              /***. BD*(   1) C  35 - C  36          0.54   10.22
0.067
 198. CR (   1) C  40              /***. RY*(   2) H  99                  0.59   11.54
0.074
 198. CR (   1) C  40              /***. RY*(   2) H 101                  0.50   11.66
0.068
 199. CR (   1) C  41              /799. RY*(   1) C  42                  0.72   11.15
0.080
 199. CR (   1) C  41              /800. RY*(   2) C  42                  0.74   10.83
0.080
 199. CR (   1) C  41              /855. RY*(   1) C  46                  0.93   11.17
0.091
 199. CR (   1) C  41              /856. RY*(   2) C  46                  0.57   10.91
0.070
 199. CR (   1) C  41              /***. BD*(   1) C  10 - N  11          1.02   10.12
0.092
 199. CR (   1) C  41              /***. BD*(   1) N  11 - C  12          0.66   10.12
0.074
 199. CR (   1) C  41              /***. BD*(   1) N  11 - C  41          0.70   10.08
0.076
 199. CR (   1) C  41              /***. BD*(   1) C  42 - C  47          0.74   10.11
0.078
 199. CR (   1) C  41              /***. BD*(   1) C  45 - C  46          0.52   10.25
0.065
 199. CR (   1) C  41              /***. BD*(   1) C  46 - C  49          0.81   10.10
0.081
 200. CR (   1) C  42              /788. RY*(   3) C  41                  0.99   11.20
0.094
 200. CR (   1) C  42              /814. RY*(   2) C  43                  0.57   10.48
0.069
 200. CR (   1) C  42              /815. RY*(   3) C  43                  0.78   10.63
0.082
 200. CR (   1) C  42              /870. RY*(   2) C  47                  0.62   10.86
0.073
 200. CR (   1) C  42              /***. BD*(   1) N  11 - C  41          0.80   10.04
0.081
 200. CR (   1) C  42              /***. BD*(   2) N  11 - C  41          5.16   10.73
0.239
 200. CR (   1) C  42              /***. BD*(   1) C  43 - C  44          0.59   10.22
0.069
 201. CR (   1) C  43              /800. RY*(   2) C  42                  1.47   10.78
0.112
 201. CR (   1) C  43              /828. RY*(   2) C  44                  1.43   10.92
0.112
 201. CR (   1) C  43              /***. RY*(   2) H  75                  0.55   11.95
0.072
 201. CR (   1) C  43              /***. BD*(   1) C  42 - C  47          0.74   10.06
0.077
 201. CR (   1) C  43              /***. BD*(   1) C  44 - C  45          0.56   10.21
0.068
 202. CR (   1) C  44              /815. RY*(   3) C  43                  0.86   10.63
0.085
 202. CR (   1) C  44              /842. RY*(   2) C  45                  1.22   10.84
0.102
 202. CR (   1) C  44              /***. BD*(   1) C  42 - C  43          0.66   10.21
0.073
 202. CR (   1) C  44              /***. BD*(   1) C  45 - C  46          0.65   10.20
0.073
 203. CR (   1) C  45              /828. RY*(   2) C  44                  1.55   10.92
0.116
 203. CR (   1) C  45              /856. RY*(   2) C  46                  1.86   10.86
0.127
 203. CR (   1) C  45              /***. BD*(   1) C  43 - C  44          0.55   10.22
0.067
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 203. CR (   1) C  45              /***. BD*(   1) C  46 - C  49           0.73   10.05
0.077
 204. CR (   1) C  46              /788. RY*(   3) C  41                  1.04   11.21
0.096
 204. CR (   1) C  46              /842. RY*(   2) C  45                  1.33   10.85
0.107
 204. CR (   1) C  46              /898. RY*(   2) C  49                  0.79   11.24
0.084
 204. CR (   1) C  46              /***. BD*(   1) N  11 - C  41          0.89   10.05
0.085
 204. CR (   1) C  46              /***. BD*(   2) N  11 - C  41          4.99   10.74
0.235
 204. CR (   1) C  46              /***. BD*(   1) C  44 - C  45          0.56   10.23
0.068
 205. CR (   1) C  47              /799. RY*(   1) C  42                  0.93   11.10
0.091
 205. CR (   1) C  47              /885. RY*(   3) C  48                  0.64   10.83
0.074
 205. CR (   1) C  47              /***. RY*(   3) C  57                  0.65   10.84
0.075
 205. CR (   1) C  47              /***. BD*(   1) C  41 - C  42          0.53   10.37
0.067
 205. CR (   1) C  47              /***. BD*(   1) C  42 - C  43          0.56   10.21
0.068
 206. CR (   1) C  48              /871. RY*(   3) C  47                  0.61   10.79
0.072
 207. CR (   1) C  49              /855. RY*(   1) C  46                  0.88   11.14
0.088
 207. CR (   1) C  49              /913. RY*(   3) C  50                  0.64   10.79
0.074
 207. CR (   1) C  49              /***. RY*(   3) C  58                  0.66   10.58
0.075
 207. CR (   1) C  49              /***. BD*(   1) C  41 - C  46          0.56   10.39
0.068
 207. CR (   1) C  49              /***. BD*(   1) C  45 - C  46          0.52   10.22
0.065
 208. CR (   1) C  50              /***. RY*(   2) H 129                   0.58   11.55
0.073
 209. CR (   1) C  51              /282. RY*(   1) C   5                  0.86   11.15
0.087
 209. CR (   1) C  51              /941. RY*(   3) C  52                  0.67   10.78
0.076
 209. CR (   1) C  51              /***. RY*(   3) C  59                  0.56   10.62
0.069
 209. CR (   1) C  51              /***. BD*(   1) C   4 - C   5          0.63   10.21
0.072
 209. CR (   1) C  51              /***. BD*(   1) C   5 - C   6          0.51   10.22
0.065
 210. CR (   1) C  52              /927. RY*(   3) C  51                  0.72   10.71
0.078
 210. CR (   1) C  52              /***. RY*(   2) H 114                   0.59   11.53
0.074
 211. CR (   1) C  53              /254. RY*(   1) C   3                  0.92   11.09
0.090
 211. CR (   1) C  53              /969. RY*(   3) C  54                  0.65   10.86
0.075
 211. CR (   1) C  53              /***. RY*(   3) C  60                  0.73   10.86
0.080
 211. CR (   1) C  53              /***. BD*(   1) C   3 - C   4          0.61   10.19
0.071
 211. CR (   1) C  53              /***. BD*(   1) C   3 - C   8          0.58   10.21
0.069
 212. CR (   1) C  54              /955. RY*(   3) C  53                  0.55   10.90
0.069
 213. CR (   1) C  55              /732. RY*(   3) C  37                  0.72   10.77
0.078
 214. CR (   1) C  56              /760. RY*(   3) C  39                  0.81   10.82
0.083
 215. CR (   1) C  57              /870. RY*(   2) C  47                  0.57   10.84
0.070
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 216. CR (   1) C  58              /899. RY*(   3) C  49                   0.60   10.70
0.072
 216. CR (   1) C  58              /***. RY*(   2) H 133                   0.60   12.10
0.076
 217. CR (   1) C  59              /927. RY*(   3) C  51                   0.54   10.71
0.068
 217. CR (   1) C  59              /***. RY*(   3) H 111                   0.55   11.53
0.071
 218. CR (   1) C  60              /954. RY*(   2) C  53                   0.71   10.82
0.078
 218. CR (   1) C  60              /***. RY*(   2) H 121                   0.61   12.11
0.077
 219. CR (   1) C  61              /620. RY*(   3) C  29                   0.66   10.76
0.075
 219. CR (   1) C  61              /***. RY*(   2) H  97                   0.58   12.14
0.075
 221. LP (   1) O   2              /226. RY*(   1) C   1                  13.44    1.59
0.131
 221. LP (   1) O   2              /232. RY*(   7) C   1                   0.82    2.98
0.045
 221. LP (   1) O   2              /***. BD*(   1) C   1 - B  14           3.25    0.91
0.049
 221. LP (   1) O   2              /***. BD*(   1) C   1 - B  15           5.86    1.02
0.070
 222. LP (   2) O   2              /228. RY*(   3) C   1                   1.64    2.41
0.060
 222. LP (   2) O   2              /230. RY*(   5) C   1                   0.82    1.06
0.028
 222. LP (   2) O   2              /***. BD*(   1) C   1 - B  14          18.75    0.49
0.089
 222. LP (   2) O   2              /***. BD*(   1) C   1 - B  15           9.06    0.61
0.070
 222. LP (   2) O   2              /***. BD*(   1) C  47 - H  80           0.61    0.51
0.017
 223. LP*(   1) B  14              /410. RY*(   3) B  14                   1.20    0.65
0.046
 223. LP*(   1) B  14              /417. RY*(  10) B  14                   0.54    1.70
0.050
 223. LP*(   1) B  14              /***. BD*(   2) C   1 - O   2         237.18    0.01
0.068
 223. LP*(   1) B  14              /***. BD*(   1) C   1 - B  14           0.60    0.30
0.020
 223. LP*(   1) B  14              /***. BD*(   1) N   9 - C  10           8.70    0.32
0.084
 223. LP*(   1) B  14              /***. BD*(   1) C  10 - N  11           8.35    0.32
0.082
 223. LP*(   1) B  14              /***. BD*(   1) B  14 - B  15           0.63    0.46
0.027
 224. LP (   1) B  15              /227. RY*(   2) C   1                   0.62    2.04
0.052
 224. LP (   1) B  15              /424. RY*(   3) B  15                   0.96    0.79
0.040
 224. LP (   1) B  15              /***. BD*(   2) C   1 - O   2         438.96    0.01
0.090
 224. LP (   1) B  15              /***. BD*(   1) C  16 - N  17           0.76    0.33
0.022
 224. LP (   1) B  15              /***. BD*(   1) C  16 - N  20           1.68    0.33
0.033
 225. LP (   1) N  20              /441. RY*(   6) C  16                   0.80    1.89
0.040
 225. LP (   1) N  20              /478. RY*(   1) C  19                   2.66    0.85
0.048
 225. LP (   1) N  20              /648. RY*(   3) C  31                   0.90    1.34
0.035
 225. LP (   1) N  20              /***. BD*(   2) C  16 - N  17          50.02    0.19
0.090
 225. LP (   1) N  20              /***. BD*(   2) C  18 - C  19          26.50    0.22
0.071
 225. LP (   1) N  20              /***. BD*(   1) C  31 - C  32           5.29    0.69
0.061
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 225. LP (   1) N  20              /***. BD*(   1) C  31 - C  36           5.28    0.70
0.061
 ***. BD*(   2) C   1 - O   2      /227. RY*(   2) C   1                  2.63    2.02
0.132
 ***. BD*(   2) C   1 - O   2      /231. RY*(   6) C   1                  1.61    0.54
0.054
 ***. BD*(   2) C   1 - O   2      /241. RY*(   2) O   2                  2.79    0.74
0.083
 ***. BD*(   2) C   1 - O   2      /247. RY*(   8) O   2                  0.52    2.94
0.071
 ***. BD*(   1) C   1 - B  14      /411. RY*(   4) B  14                  0.70    0.88
0.094
 ***. BD*(   1) C   1 - B  14      /***. BD*(   1) C   1 - O   2          0.72    0.18
0.037
 ***. BD*(   1) C   1 - B  14      /***. BD*(   1) C  10 - N  11          1.07    0.01
0.012
 ***. BD*(   1) C   1 - B  14      /***. BD*(   1) B  14 - B  15          3.51    0.15
0.075
 ***. BD*(   1) C   1 - B  14      /***. BD*(   1) C  16 - N  20          0.65    0.02
0.011
 ***. BD*(   1) C   1 - B  14      /***. BD*(   1) C  47 - H  80          0.53    0.02
0.012
 ***. BD*(   1) C   1 - B  14      /***. BD*(   1) C  55 - H 110          0.57    0.01
0.010
 ***. BD*(   1) C   1 - B  14      /***. BD*(   1) C  58 - H 133          0.58    0.01
0.010
 ***. BD*(   2) C   3 - C   8      /326. RY*(   3) C   8                  1.18    0.71
0.063
 ***. BD*(   2) C   3 - C   8      /***. BD*(   1) C  53 - C  54          1.65    0.28
0.046
 ***. BD*(   2) C   3 - C   8      /***. BD*(   1) C  53 - C  60          0.62    0.30
0.029
 ***. BD*(   2) C   4 - C   5      /223. LP*(   1) B  14                  3.85    0.02
0.011
 ***. BD*(   2) C   4 - C   5      /269. RY*(   2) C   4                  0.57    0.74
0.042
 ***. BD*(   2) C   4 - C   5      /298. RY*(   3) C   6                  0.64    0.53
0.038
 ***. BD*(   2) C   4 - C   5      /***. BD*(   1) N   9 - C  10          1.57    0.34
0.045
 ***. BD*(   2) C   4 - C   5      /***. BD*(   1) N   9 - C  13          1.46    0.33
0.044
 ***. BD*(   2) C   4 - C   5      /***. BD*(   1) C  51 - C  52          1.35    0.27
0.039
 ***. BD*(   2) C   4 - C   5      /***. BD*(   1) C  51 - C  59          1.38    0.28
0.040
 ***. BD*(   2) C   6 - C   7      /298. RY*(   3) C   6                  0.97    0.54
0.050
 ***. BD*(   2) C   6 - C   7      /312. RY*(   3) C   7                  1.84    0.54
0.069
 ***. BD*(   2) N   9 - C  10      /223. LP*(   1) B  14                  0.85    0.07
0.009
 ***. BD*(   2) N   9 - C  10      /353. RY*(   2) C  10                  2.17    1.51
0.085
 ***. BD*(   2) N   9 - C  10      /355. RY*(   4) C  10                  0.79    1.63
0.053
 ***. BD*(   2) N   9 - C  10      /***. BD*(   1) C   1 - B  14          6.21    0.38
0.067
 ***. BD*(   2) N   9 - C  10      /***. BD*(   1) C   3 - C   4          1.04    0.50
0.033
 ***. BD*(   2) N   9 - C  10      /***. BD*(   1) C   4 - C   5          1.34    0.50
0.038
 ***. BD*(   2) N   9 - C  10      /***. BD*(   2) C  12 - C  13         23.04    0.03
0.035
 ***. BD*(   2) N   9 - C  10      /***. BD*(   1) B  14 - B  15          1.29    0.53
0.038
 ***. BD*(   2) N  11 - C  41      /226. RY*(   1) C   1                  0.68    0.02
0.006
 ***. BD*(   2) N  11 - C  41      /257. RY*(   4) C   3                  0.86    0.04
0.011
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 ***. BD*(   2) N  11 - C  41        /372. RY*(   7) N  11                    1.35    1.41
0.082
 ***. BD*(   2) N  11 - C  41        /409. RY*(   2) B  14                    0.63    0.13
0.017
 ***. BD*(   2) N  11 - C  41        /411. RY*(   4) B  14                    0.85    0.22
0.025
 ***. BD*(   2) N  11 - C  41        /788. RY*(   3) C  41                   51.35    0.47
0.291
 ***. BD*(   2) N  11 - C  41        /789. RY*(   4) C  41                   20.91    0.61
0.211
 ***. BD*(   2) N  11 - C  41        /790. RY*(   5) C  41                    3.41    0.74
0.094
 ***. BD*(   2) N  11 - C  41        /792. RY*(   7) C  41                    9.88    0.59
0.143
 ***. BD*(   2) N  11 - C  41        /793. RY*(   8) C  41                    3.99    0.61
0.092
 ***. BD*(   2) N  11 - C  41        /794. RY*(   9) C  41                   85.13    0.80
0.489
 ***. BD*(   2) N  11 - C  41        /799. RY*(   1) C  42                    0.60    0.37
0.028
 ***. BD*(   2) N  11 - C  41        /800. RY*(   2) C  42                   21.69    0.06
0.066
 ***. BD*(   2) N  11 - C  41        /802. RY*(   4) C  42                  132.45    0.02
0.088
 ***. BD*(   2) N  11 - C  41        /805. RY*(   7) C  42                    3.22    0.85
0.098
 ***. BD*(   2) N  11 - C  41        /808. RY*(  10) C  42                    0.56    1.40
0.052
 ***. BD*(   2) N  11 - C  41        /809. RY*(  11) C  42                    3.94    1.33
0.135
 ***. BD*(   2) N  11 - C  41        /811. RY*(  13) C  42                    1.44    1.40
0.084
 ***. BD*(   2) N  11 - C  41        /813. RY*(   1) C  43                    0.94    0.43
0.037
 ***. BD*(   2) N  11 - C  41        /816. RY*(   4) C  43                    3.35    0.32
0.061
 ***. BD*(   2) N  11 - C  41        /819. RY*(   7) C  43                    0.78    0.76
0.046
 ***. BD*(   2) N  11 - C  41        /824. RY*(  12) C  43                    0.69    1.06
0.051
 ***. BD*(   2) N  11 - C  41        /828. RY*(   2) C  44                    2.11    0.19
0.038
 ***. BD*(   2) N  11 - C  41        /832. RY*(   6) C  44                    0.98    1.42
0.070
 ***. BD*(   2) N  11 - C  41        /835. RY*(   9) C  44                    0.79    0.11
0.017
 ***. BD*(   2) N  11 - C  41        /842. RY*(   2) C  45                    4.76    0.11
0.043
 ***. BD*(   2) N  11 - C  41        /844. RY*(   4) C  45                    3.37    0.32
0.062
 ***. BD*(   2) N  11 - C  41        /848. RY*(   8) C  45                    0.80    0.62
0.042
 ***. BD*(   2) N  11 - C  41        /850. RY*(  10) C  45                    0.57    0.48
0.031
 ***. BD*(   2) N  11 - C  41        /853. RY*(  13) C  45                    0.70    1.53
0.061
 ***. BD*(   2) N  11 - C  41        /855. RY*(   1) C  46                    3.36    0.40
0.068
 ***. BD*(   2) N  11 - C  41        /856. RY*(   2) C  46                    9.01    0.14
0.066
 ***. BD*(   2) N  11 - C  41        /860. RY*(   6) C  46                    0.67    0.77
0.043
 ***. BD*(   2) N  11 - C  41        /861. RY*(   7) C  46                    1.05    0.78
0.054
 ***. BD*(   2) N  11 - C  41        /864. RY*(  10) C  46                    0.57    1.18
0.048
 ***. BD*(   2) N  11 - C  41        /865. RY*(  11) C  46                    2.79    1.45
0.119
 ***. BD*(   2) N  11 - C  41        /866. RY*(  12) C  46                    1.40    0.58
0.054
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***. BD*(2) N 11 - C 41	/867. RY*(13) C 46	2.37	1.45	0.110
***. BD*(2) N 11 - C 41	/869. RY*(1) C 47	3.62	0.06	0.026
***. BD*(2) N 11 - C 41	/870. RY*(2) C 47	4.69	0.13	0.046
***. BD*(2) N 11 - C 41	/871. RY*(3) C 47	1.04	0.08	0.017
***. BD*(2) N 11 - C 41	/890. RY*(8) C 48	0.51	0.79	0.038
***. BD*(2) N 11 - C 41	/897. RY*(1) C 49	1.81	0.12	0.027
***. BD*(2) N 11 - C 41	/898. RY*(2) C 49	1.02	0.51	0.043
***. BD*(2) N 11 - C 41	/902. RY*(6) C 49	0.63	0.19	0.021
***. BD*(2) N 11 - C 41	/903. RY*(7) C 49	0.88	1.02	0.056
***. BD*(2) N 11 - C 41	/907. RY*(11) C 49	0.99	0.94	0.057
***. BD*(2) N 11 - C 41	/913. RY*(3) C 50	1.46	0.04	0.015
***. BD*(2) N 11 - C 41	/***. RY*(8) C 58	0.71	0.38	0.031
***. BD*(2) N 11 - C 41	/***. RY*(1) H 127	1.27	0.09	0.019
***. BD*(2) C 12 - C 13	/384. RY*(5) C 12	0.54	1.78	0.074
***. BD*(2) C 12 - C 13	/398. RY*(5) C 13	0.53	1.78	0.073
***. BD*(2) C 16 - N 17	/223. LP*(1) B 14	1.11	0.09	0.011
***. BD*(2) C 16 - N 17	/224. LP (1) B 15	68.17	0.09	0.083
***. BD*(2) C 16 - N 17	/437. RY*(2) C 16	1.61	1.30	0.074
***. BD*(2) C 16 - N 17	/438. RY*(3) C 16	1.00	1.51	0.063
***. BD*(2) C 16 - N 17	/***. BD*(2) C 18 - C 19	28.64	0.03	0.037
***. BD*(2) C 16 - N 17	/***. BD*(1) C 21 - C 22	0.95	0.51	0.035
***. BD*(2) C 16 - N 17	/***. BD*(1) C 21 - C 26	1.10	0.51	0.037
***. BD*(2) C 18 - C 19	/468. RY*(5) C 18	0.53	1.77	0.072
***. BD*(2) C 18 - C 19	/482. RY*(5) C 19	0.51	1.77	0.072
***. BD*(2) C 21 - C 26	/507. RY*(2) C 21	0.58	0.75	0.042
***. BD*(2) C 21 - C 26	/564. RY*(3) C 25	0.63	0.56	0.038
***. BD*(2) C 21 - C 26	/***. BD*(1) C 16 - N 17	1.55	0.35	0.044
***. BD*(2) C 21 - C 26	/***. BD*(1) N 17 - C 18	1.48	0.33	0.043
***. BD*(2) C 21 - C 26	/***. BD*(1) C 29 - C 30	1.41	0.27	0.039
***. BD*(2) C 21 - C 26	/***. BD*(1) C 29 - C 61	1.42	0.28	0.040
***. BD*(2) C 22 - C 23	/536. RY*(3) C 23	0.84	0.83	0.058
***. BD*(2) C 22 - C 23	/***. BD*(1) C 27 - C 28	1.64	0.27	0.045
***. BD*(2) C 22 - C 23	/***. BD*(1) C 27 - C 62	0.59	0.29	0.028
***. BD*(2) C 24 - C 25	/550. RY*(3) C 24	2.03	0.57	0.074
***. BD*(2) C 24 - C 25	/564. RY*(3) C 25	0.98	0.57	0.051

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 ***. BD*(   2) C  31 - C  36        /647. RY*(   2) C  31                    0.60    0.74
0.043
 ***. BD*(   2) C  31 - C  36        /704. RY*(   3) C  35                    0.52    0.58
0.036
 ***. BD*(   2) C  31 - C  36        /***. BD*(   1) C  16 - N  20            1.49    0.35
0.044
 ***. BD*(   2) C  31 - C  36        /***. BD*(   1) C  19 - N  20            1.42    0.33
0.043
 ***. BD*(   2) C  31 - C  36        /***. BD*(   1) C  39 - C  40            1.46    0.28
0.041
 ***. BD*(   2) C  31 - C  36        /***. BD*(   1) C  39 - C  56            1.16    0.29
0.037
 ***. BD*(   2) C  32 - C  33        /676. RY*(   3) C  33                    1.07    0.73
0.061
 ***. BD*(   2) C  32 - C  33        /***. BD*(   1) C  37 - C  38            1.17    0.28
0.038
 ***. BD*(   2) C  32 - C  33        /***. BD*(   1) C  37 - C  55            1.56    0.28
0.044
 ***. BD*(   2) C  34 - C  35        /690. RY*(   3) C  34                    1.89    0.60
0.074
 ***. BD*(   2) C  34 - C  35        /704. RY*(   3) C  35                    1.03    0.59
0.054
 ***. BD*(   2) C  41 - C  46        /787. RY*(   2) C  41                    0.90    0.76
0.054
 ***. BD*(   2) C  41 - C  46        /788. RY*(   3) C  41                    0.61    1.44
0.061
 ***. BD*(   2) C  41 - C  46        /843. RY*(   3) C  45                    0.66    0.50
0.037
 ***. BD*(   2) C  41 - C  46        /***. BD*(   1) C  10 - N  11            1.64    0.32
0.045
 ***. BD*(   2) C  41 - C  46        /***. BD*(   1) N  11 - C  12            1.52    0.31
0.044
 ***. BD*(   2) C  41 - C  46        /***. BD*(   2) N  11 - C  41            9.60    0.97
0.134
 ***. BD*(   2) C  41 - C  46        /***. BD*(   1) C  41 - C  42            1.49    0.61
0.060
 ***. BD*(   2) C  41 - C  46        /***. BD*(   1) C  41 - C  46            1.33    0.61
0.057
 ***. BD*(   2) C  41 - C  46        /***. BD*(   1) C  49 - C  50            1.48    0.26
0.039
 ***. BD*(   2) C  41 - C  46        /***. BD*(   1) C  49 - C  58            1.38    0.26
0.038
 ***. BD*(   2) C  42 - C  43        /814. RY*(   2) C  43                    0.84    0.73
0.054
 ***. BD*(   2) C  42 - C  43        /815. RY*(   3) C  43                    0.50    0.89
0.046
 ***. BD*(   2) C  42 - C  43        /***. BD*(   2) C  41 - C  46          154.33    0.01
0.068
 ***. BD*(   2) C  42 - C  43        /***. BD*(   1) C  47 - C  48            1.65    0.28
0.046
 ***. BD*(   2) C  42 - C  43        /***. BD*(   1) C  47 - C  57            0.53    0.29
0.027
 ***. BD*(   2) C  44 - C  45        /829. RY*(   3) C  44                    1.93    0.57
0.072
 ***. BD*(   2) C  44 - C  45        /843. RY*(   3) C  45                    1.01    0.52
0.050
 ***. BD*(   2) C  44 - C  45        /***. BD*(   2) C  41 - C  46           94.77    0.02
0.069
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Natural Bond Orbitals (Summary):

NBO	Occupancy	Energy	Principal Delocalizations (geminal,vicinal,remote)
Molecular unit 1 (C55H72B2N4O)			
1. BD (1) C 1 - O 2	1.99525	-0.90192	1456(g),1455(g),226(g) 422(v)
2. BD (2) C 1 - O 2	1.98559	-0.25985	224(v),223(v),1454(g)
3. BD (1) C 1 - B 14	1.68991	-0.31855	1485(v),1473(v),1456(g) 1484(g),1455(g),240(v)

						242(v),224(v),1472(v),229(g)
4.	BD (	1) C	1 - B	15	1.86978	-0.40234 1476(v),1455(g),1488(v) 1484(g),1485(g),223(v) 1453(g),240(v),242(v),430(g) 436(v),1456(g),1487(v) 413(v),433(g)
5.	BD (	1) C	3 - C	4	1.96959	-0.62652 1465(v),1471(v),1461(g) 1474(v),1472(v),1458(g) 1582(v),1473(v),338(v) 283(v),1460(g)
6.	BD (	1) C	3 - C	8	1.97359	-0.62621 1463(v),1470(v),1469(g) 1457(g),311(v),268(v) 1583(v),1460(g),953(v)
7.	BD (	2) C	3 - C	8	1.63548	-0.21626 1467(v),1462(v),1581(v) 312(v),1582(v),1583(v)
8.	BD (	1) C	3 - C	53	1.96975	-0.54124 1461(v),1469(v),268(v) 1584(v),1602(v),324(v) 1458(g),1457(g)
9.	BD (	1) C	4 - C	5	1.96881	-0.63017 1460(v),1468(v),1457(g) 1472(v),1464(g),1473(v) 255(v),338(v),1474(v) 1576(v),1465(g),1575(v) 297(v)
10.	BD (	2) C	4 - C	5	1.66564	-0.22340 1459(v),1467(v),1472(v) 1474(v),1576(v),1575(v) 298(v)
11.	BD (	1) C	4 - N	9	1.98185	-0.70909 1458(v),1464(v),1475(v) 1480(v),1472(g),352(v) 254(v),395(v),1457(g),282(v) 1474(g),1461(g)
12.	BD (	1) C	5 - C	6	1.97300	-0.62857 1463(v),1470(v),1466(g) 1461(g),1577(v),311(v) 268(v),925(v),1465(g)
13.	BD (	1) C	5 - C	51	1.96978	-0.55083 1457(v),1466(v),268(v) 1578(v),1599(v),296(v) 1461(g),1464(g)
14.	BD (	1) C	6 - C	7	1.98099	-0.63543 1465(v),1471(v),1464(g) 1469(g),282(v),325(v),324(v)
15.	BD (	2) C	6 - C	7	1.67366	-0.22235 1462(v),1459(v)
16.	BD (	1) C	6 - H	78	1.97545	-0.45586 1461(v),1469(v),282(v) 310(v)
17.	BD (	1) C	7 - C	8	1.98085	-0.63266 1460(v),1468(v),1458(g) 1466(g),254(v),297(v)
18.	BD (	1) C	7 - H	77	1.97757	-0.45528 1458(v),1464(v),324(v) 296(v),1168(r)
19.	BD (	1) C	8 - H	76	1.97490	-0.45077 1457(v),1466(v),254(v) 310(v)
20.	BD (	1) N	9 - C	10	1.97311	-0.71918 1478(v),1483(v),1476(g) 1462(v),1484(v),223(v) 1463(g),269(v),1474(g) 1461(v),396(v),1457(v)
21.	BD (	2) N	9 - C	10	1.85857	-0.28652 1481(v),1461(v),1457(v) 394(v),1455(v),270(v) 1484(v)
22.	BD (	1) N	9 - C	13	1.97621	-0.71960 1482(v),1476(v),1462(v) 1457(v),382(v),1472(g) 1463(g),269(v),1478(r) 1480(g),354(v),352(v) 1475(v),355(v)
23.	BD (	1) C	10 - N	11	1.97446	-0.72168 1463(v),1482(v),1476(g) 1478(g),1477(g),1551(v) 787(v),1484(v),1550(v) 382(v),223(v)
24.	BD (	1) C	10 - B	14	1.96616	-0.51296 1474(v),1477(v),1484(g) 422(v),1472(g),1475(g) 1456(v),416(g),367(v),413(g) 1455(g),1485(v),339(v) 338(v),414(g),411(g),419(g) 366(v)
25.	BD (	1) N	11 - C	12	1.97540	-0.71724 1483(v),1476(v),1551(v) 354(v),1549(v),1475(g)

					396(v),1478(g),352(v)
					1463(r),1472(v),787(v)
					1480(g)
26. BD (	1) N	11 - C	41	1.98143	-0.70796 1552(v),1560(v),1472(v)
					1480(v),1475(g),1479(g)
					352(v),799(v),1550(g),381(v)
					855(v),1477(g)
27. BD (	2) N	11 - C	41	1.60454	-0.22954 1473(v),1481(v),1550(g)
					1549(g),380(v),1479(g)
					1551(g),358(v),794(g),788(g)
					1560(v),1552(v)
28. BD (	1) C	12 - C	13	1.97682	-0.66846 1463(v),1478(v),367(v)
					339(v),1483(g),1482(g)
29. BD (	2) C	12 - C	13	1.91018	-0.24724 1473(v)
30. BD (	1) C	12 - H	71	1.97879	-0.49868 1475(v),1474(v),367(v)
					395(v),1480(g)
31. BD (	1) C	13 - H	72	1.97878	-0.49877 1472(v),1477(v),339(v)
					381(v),1480(g)
32. BD (	1) B	14 - B	15	1.82710	-0.28824 1453(v),1486(v),1485(g)
					1455(g),1456(g),352(v)
					436(v),1476(g),408(g)
					1475(v),1473(v),355(v)
					1472(v),226(v),356(v),419(g)
					432(g),422(g),411(g),438(v)
33. BD (	1) B	15 - C	16	1.95720	-0.50897 1484(g),1489(v),1494(v)
					408(v),1456(g),1476(v)
					1453(v),450(v),492(v)
					1455(v),1488(g),1486(g)
					430(g),433(g),436(g),452(v)
34. BD (	1) C	16 - N	17	1.97511	-0.74754 1496(v),1493(v),1485(g)
					1489(g),1490(g),1484(v)
					1499(v),507(v),1498(v)
					466(v),492(v),1497(v)
35. BD (	2) C	16 - N	17	1.85625	-0.30884 1492(v),224(v),1497(v)
					1498(v),464(v),508(v)
36. BD (	1) C	16 - N	20	1.97558	-0.75212 1490(v),1495(v),1485(g)
					1494(g),1496(g),1525(v)
					647(v),480(v),1523(v),450(v)
					1524(v)
37. BD (	1) N	17 - C	18	1.97731	-0.74361 1495(v),1485(v),1499(v)
					439(v),1486(g),1490(g)
					1497(v),436(v),480(v)
					1496(r),507(v),1488(v)
					1491(g)
38. BD (	1) N	17 - C	21	1.98138	-0.71684 1500(v),1508(v),1488(v)
					1486(g),436(v),1491(v)
					465(v),520(v),1489(g),576(v)
					1497(g)
39. BD (	1) C	18 - C	19	1.97697	-0.68216 1490(v),1496(v),450(v)
					492(v),1495(g),1493(g)
40. BD (	2) C	18 - C	19	1.87142	-0.26470 1487(v)
41. BD (	1) C	18 - H	63	1.97977	-0.51490 1486(v),1494(v),450(v)
					479(v),1491(g)
42. BD (	1) C	19 - N	20	1.97686	-0.74244 1493(v),1485(v),1525(v)
					1488(g),436(v),1496(g)
					466(v),1524(v),438(v)
					1490(r),647(v),1486(v)
					1491(g)
43. BD (	1) C	19 - H	64	1.98034	-0.51517 1488(v),1489(v),492(v)
					465(v),1491(g)
44. BD (	1) N	20 - C	31	1.98185	-0.72487 1534(v),1526(v),1486(v)
					1488(g),436(v),1491(v)
					479(v),716(v),1494(g)
					1524(g),660(v),1523(g)
45. BD (	1) C	21 - C	22	1.96835	-0.63096 1510(v),1504(v),1498(g)
					1486(v),1500(g),1512(v)
					1489(v),1487(v),578(v)
					451(v),1502(g)
46. BD (	1) C	21 - C	26	1.96787	-0.63406 1502(v),1509(v),1497(g)
					1486(v),1508(g),1487(v)
					451(v),522(v),1489(v)

							1510(g),1517(v),1518(v)
47.	BD	(2)	C	21 - C	26	1.67376	-0.22594 1501(v),1506(v),1486(v) 1489(v),1518(v),1517(v) 564(v),521(v)
48.	BD	(1)	C	22 - C	23	1.97239	-0.62672 1490(v),1507(v),1503(g) 1497(g),549(v),506(v) 1513(v),1502(g),590(v)
49.	BD	(2)	C	22 - C	23	1.63022	-0.21455 1506(v),1499(v),1511(v) 1513(v),550(v),1512(v)
50.	BD	(1)	C	22 - C	27	1.96962	-0.54713 1498(v),1503(v),1514(v) 506(v),1608(v),534(v) 1500(g),1497(g)
51.	BD	(1)	C	23 - C	24	1.98062	-0.63148 1502(v),1509(v),1500(g) 1505(g),520(v),563(v)
52.	BD	(1)	C	23 - H	67	1.97434	-0.44961 1497(v),1505(v),520(v) 548(v)
53.	BD	(1)	C	24 - C	25	1.98089	-0.63462 1510(v),1504(v),1508(g) 1503(g),576(v),535(v),534(v)
54.	BD	(2)	C	24 - C	25	1.66929	-0.22093 1499(v),1501(v)
55.	BD	(1)	C	24 - H	66	1.97747	-0.45366 1508(v),1500(v),534(v) 562(v),1113(r),1103(r)
56.	BD	(1)	C	25 - C	26	1.97185	-0.62917 1490(v),1507(v),1498(g) 1505(g),1519(v),549(v) 506(v),618(v),1510(g)
57.	BD	(1)	C	25 - H	65	1.97514	-0.45543 1498(v),1503(v),576(v) 548(v)
58.	BD	(1)	C	26 - C	29	1.96965	-0.55319 1497(v),1505(v),506(v) 1520(v),1605(v),562(v) 1508(g),1498(g)
59.	BD	(1)	C	27 - C	28	1.97151	-0.52757 1501(v),1610(v),1497(v) 1500(v),521(v),1079(v)
60.	BD	(1)	C	27 - C	62	1.97918	-0.52407 1497(v),1515(v),1501(v) 1502(g)
61.	BD	(1)	C	27 - H	84	1.95937	-0.41115 1500(v),1609(v),1516(v) 1501(v)
62.	BD	(1)	C	28 - H	90	1.98583	-0.43361 1502(v)
63.	BD	(1)	C	28 - H	91	1.98733	-0.43809 1512(v)
64.	BD	(1)	C	28 - H	92	1.98896	-0.43441 1513(v)
65.	BD	(1)	C	29 - C	30	1.97625	-0.53808 1499(v),1498(v),1606(v) 577(v),1510(g)
66.	BD	(1)	C	29 - C	61	1.97478	-0.53465 1499(v),1498(v),1522(v) 1510(g)
67.	BD	(1)	C	29 - H	83	1.96477	-0.42514 1508(v),1607(v),1521(v)
68.	BD	(1)	C	30 - H	93	1.98638	-0.44097 1510(v)
69.	BD	(1)	C	30 - H	94	1.98825	-0.44229 1519(v)
70.	BD	(1)	C	30 - H	95	1.98830	-0.44198 1518(v)
71.	BD	(1)	C	31 - C	32	1.96778	-0.64047 1536(v),1530(v),1524(g) 1488(v),1526(g),717(v) 1537(v),1494(v),493(v) 1528(g)
72.	BD	(1)	C	31 - C	36	1.96880	-0.64149 1528(v),1535(v),1523(g) 1488(v),1534(g),1494(v) 1544(v),493(v),1536(g) 661(v),703(v),1543(v)
73.	BD	(2)	C	31 - C	36	1.65932	-0.23277 1527(v),1532(v),1488(v) 1494(v),1543(v),1544(v) 704(v)
74.	BD	(1)	C	32 - C	33	1.97272	-0.63809 1496(v),1533(v),1529(g) 1523(g),1539(v),689(v) 646(v),730(v),1528(g)
75.	BD	(2)	C	32 - C	33	1.64228	-0.22841 1532(v),1525(v),1538(v) 1537(v),690(v)
76.	BD	(1)	C	32 - C	37	1.97001	-0.55922 1524(v),1529(v),646(v) 1587(v),1540(v),674(v) 1526(g),1523(g)
77.	BD	(1)	C	33 - C	34	1.98090	-0.64364 1528(v),1535(v),1526(g) 1531(g),660(v),703(v)
78.	BD	(1)	C	33 - H	70	1.97515	-0.46347 1523(v),1531(v),660(v) 688(v)
79.	BD	(1)	C	34 - C	35	1.98086	-0.64383 1536(v),1530(v),1534(g) 1529(g),716(v)

80. BD (2) C 34 - C 35	1.66541	-0.23018	1525(v),1527(v)
81. BD (1) C 34 - H 69	1.97730	-0.46349	1534(v),1526(v),702(v) 674(v),1128(r),1118(r)
82. BD (1) C 35 - C 36	1.97274	-0.63694	1496(v),1533(v),1524(g) 1531(g),1545(v),689(v) 646(v),1536(g),758(v)
83. BD (1) C 35 - H 68	1.97505	-0.46194	1524(v),1529(v),716(v) 688(v)
84. BD (1) C 36 - C 39	1.96945	-0.55598	1523(v),1531(v),646(v) 1546(v),1590(v),702(v) 1534(g),1524(g)
85. BD (1) C 37 - C 38	1.97786	-0.54302	1523(v),1527(v),1589(v) 661(v),1528(g)
86. BD (1) C 37 - C 55	1.97252	-0.53746	1527(v),1523(v),1541(v) 662(v),1528(g),744(v)
87. BD (1) C 37 - H 85	1.96378	-0.42874	1526(v),1542(v),1588(v)
88. BD (1) C 38 - H 105	1.98608	-0.44367	1528(v)
89. BD (1) C 38 - H 106	1.98876	-0.44508	1538(v)
90. BD (1) C 38 - H 107	1.98837	-0.44651	1539(v)
91. BD (1) C 39 - C 40	1.97424	-0.53674	1525(v),1524(v),1591(v) 718(v),1536(g)
92. BD (1) C 39 - C 56	1.97484	-0.53277	1524(v),1525(v),1548(v) 1536(g)
93. BD (1) C 39 - H 86	1.96388	-0.42166	1534(v),1592(v),1547(v)
94. BD (1) C 40 - H 99	1.98600	-0.43985	1536(v)
95. BD (1) C 40 - H 100	1.98848	-0.44199	1545(v)
96. BD (1) C 40 - H 101	1.98843	-0.44171	1544(v)
97. BD (1) C 41 - C 42	1.75785	-0.40643	1479(g),1550(g),1549(g) 794(g),1551(g),788(g),789(g) 1556(v),1562(v),792(g) 1475(v),1564(v),1477(v) 809(g),861(v),855(v),787(g) 800(g),816(v),802(g),865(v) 790(g),1560(v),805(g),867(v) 815(v),1554(g),793(g),814(v)
98. BD (1) C 41 - C 46	1.74502	-0.39338	1479(g),1549(g),1550(g) 794(g),1551(g),788(g),789(g) 1561(v),1554(v),1475(v) 792(g),858(g),842(v),805(v) 1478(g),787(g),865(g),844(v) 855(g),856(g),1570(v) 1569(v),809(v),1552(v) 1562(g),898(v),1477(v) 793(g),790(g),867(g),799(v) 811(v),902(v)
99. BD (2) C 41 - C 46	1.64949	-0.20314	1479(g),1553(v),1558(v) 1549(g),1550(g),1475(v) 1477(v),794(g),1569(v) 1570(v),1551(g),843(v) 788(g),789(g)
100. BD (1) C 42 - C 43	1.97345	-0.62639	1478(v),1559(v),1555(g) 1549(g),1479(v),828(v) 786(v),1565(v),1554(g) 869(v)
101. BD (2) C 42 - C 43	1.63619	-0.21701	1558(v),1551(v),1563(v) 829(v),1565(v),1564(v)
102. BD (1) C 42 - C 47	1.96988	-0.54167	1479(v),1555(v),1550(v) 786(v),1566(v),1593(v) 813(v),1552(g)
103. BD (1) C 43 - C 44	1.98096	-0.63321	1554(v),1561(v),1552(g) 1557(g),799(v),842(v)
104. BD (1) C 43 - H 75	1.97475	-0.45107	1557(v),1549(v),799(v) 827(v)
105. BD (1) C 44 - C 45	1.98096	-0.63649	1562(v),1556(v),1560(g) 1555(g),855(v),813(v)
106. BD (2) C 44 - C 45	1.67441	-0.22311	1551(v),1553(v)
107. BD (1) C 44 - H 74	1.97752	-0.45579	1560(v),1552(v),841(v) 813(v),1153(r),1143(r)
108. BD (1) C 45 - C 46	1.97278	-0.62913	1478(v),1559(v),1550(g) 1557(g),1571(v),1479(v) 828(v),786(v),897(v),1562(g)

109. BD (1) C 45 - H 73	1.97534	-0.45630	1555(v),1550(v),855(v) 827(v)
110. BD (1) C 46 - C 49	1.96959	-0.55162	1479(v),1557(v),1549(v) 786(v),1572(v),1596(v) 841(v),1560(g)
111. BD (1) C 47 - C 48	1.96910	-0.51752	1553(v),1595(v),1552(v) 801(v),1549(v),1009(v)
112. BD (1) C 47 - C 57	1.97975	-0.51944	1549(v),1567(v),800(v) 1553(v),1554(g)
113. BD (1) C 47 - H 80	1.95741	-0.39872	1552(v),1594(v),1568(v) 1553(v)
114. BD (1) C 48 - H 126	1.98559	-0.42435	1554(v)
115. BD (1) C 48 - H 127	1.98706	-0.42894	1564(v)
116. BD (1) C 48 - H 128	1.98982	-0.42719	1565(v)
117. BD (1) C 49 - C 50	1.97532	-0.53535	1551(v),1550(v),1597(v) 857(v),1562(g)
118. BD (1) C 49 - C 58	1.97545	-0.53411	1551(v),1550(v),1574(v) 1562(g)
119. BD (1) C 49 - H 79	1.96417	-0.42156	1560(v),1598(v),1573(v)
120. BD (1) C 50 - H 129	1.98629	-0.43880	1562(v)
121. BD (1) C 50 - H 130	1.98839	-0.44053	1571(v)
122. BD (1) C 50 - H 131	1.98804	-0.43970	1570(v)
123. BD (1) C 51 - C 52	1.97541	-0.53517	1462(v),1461(v),1601(v) 283(v),1465(g)
124. BD (1) C 51 - C 59	1.97561	-0.53506	1462(v),1461(v),1579(v) 284(v),1465(g)
125. BD (1) C 51 - H 81	1.96408	-0.42206	1464(v),1600(v),1580(v)
126. BD (1) C 52 - H 114	1.98624	-0.43889	1465(v)
127. BD (1) C 52 - H 115	1.98831	-0.43949	1576(v)
128. BD (1) C 52 - H 116	1.98844	-0.44074	1577(v)
129. BD (1) C 53 - C 54	1.96921	-0.51830	1459(v),1603(v),1457(v) 256(v),1458(v)
130. BD (1) C 53 - C 60	1.97956	-0.51874	1457(v),1586(v),1459(v) 255(v),1460(g)
131. BD (1) C 53 - H 82	1.95860	-0.40000	1458(v),1604(v),1585(v) 1459(v)
132. BD (1) C 54 - H 117	1.98561	-0.42530	1460(v)
133. BD (1) C 54 - H 118	1.98955	-0.42769	1583(v)
134. BD (1) C 54 - H 119	1.98730	-0.42974	1582(v)
135. BD (1) C 55 - H 108	1.98449	-0.43488	1528(v)
136. BD (1) C 55 - H 109	1.98741	-0.43738	1539(v)
137. BD (1) C 55 - H 110	1.98644	-0.43170	1537(v)
138. BD (1) C 56 - H 102	1.98436	-0.42720	1536(v)
139. BD (1) C 56 - H 103	1.98632	-0.42387	1543(v)
140. BD (1) C 56 - H 104	1.98716	-0.43095	1545(v)
141. BD (1) C 57 - H 123	1.98474	-0.41620	1554(v)
142. BD (1) C 57 - H 124	1.98872	-0.42463	1565(v)
143. BD (1) C 57 - H 125	1.98684	-0.41864	1563(v)
144. BD (1) C 58 - H 132	1.98532	-0.43377	1562(v)
145. BD (1) C 58 - H 133	1.98713	-0.43197	1569(v)
146. BD (1) C 58 - H 134	1.98795	-0.43674	1571(v)
147. BD (1) C 59 - H 111	1.98540	-0.43476	1465(v)
148. BD (1) C 59 - H 112	1.98797	-0.43734	1577(v)
149. BD (1) C 59 - H 113	1.98638	-0.43257	1575(v)
150. BD (1) C 60 - H 120	1.98440	-0.41192	1460(v)
151. BD (1) C 60 - H 121	1.98692	-0.41430	1581(v)
152. BD (1) C 60 - H 122	1.98826	-0.42173	1583(v)
153. BD (1) C 61 - H 96	1.98496	-0.43294	1510(v)
154. BD (1) C 61 - H 97	1.98679	-0.43018	1517(v)
155. BD (1) C 61 - H 98	1.98764	-0.43495	1519(v)
156. BD (1) C 62 - H 87	1.98463	-0.42022	1502(v)
157. BD (1) C 62 - H 88	1.98761	-0.42450	1513(v)
158. BD (1) C 62 - H 89	1.98595	-0.41384	1511(v)
159. CR (1) C 1	1.99867	-9.74357	1485(v),1456(g),1453(g) 1455(g),243(v),1476(v)
160. CR (1) O 2	1.99981	-18.41443	226(v),1456(v),1455(v)
161. CR (1) C 3	1.99898	-9.73478	325(v),270(v),1461(v) 1463(v),1469(v)
162. CR (1) C 4	1.99875	-9.77349	1472(v),282(v),1465(v) 254(v),1460(v),1474(v) 1463(g),255(v),1457(g)

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                                                    1461(g),1464(v)
163. CR (   1) C   5                 1.99898    -9.73872  297(v),270(v),1463(v)
                                                    1457(v),926(v),1466(v)
164. CR (   1) C   6                 1.99910    -9.72728  311(v),283(v),284(v),1465(v)
                                                    1461(v),1469(v),1169(v)
165. CR (   1) C   7                 1.99920    -9.73058  297(v),325(v),1458(v)
                                                    1464(v)
166. CR (   1) C   8                 1.99910    -9.72423  255(v),311(v),1460(v)
                                                    1466(v),1457(v)
167. CR (   1) N   9                 1.99944   -13.85327  396(v),268(v),1476(v)
168. CR (   1) C  10                 1.99868    -9.79369  1484(v),1476(g),1478(v)
                                                    1463(v),408(v),411(v)
                                                    1474(v),1477(v)
169. CR (   1) N  11                 1.99943   -13.85487  354(v),382(v),786(v),1476(v)
170. CR (   1) C  12                 1.99903    -9.77424  1480(g),1478(v),395(v)
                                                    1483(v),396(v),368(v)
                                                    1475(v),1133(v)
171. CR (   1) C  13                 1.99902    -9.77405  1463(v),1480(g),382(v)
                                                    1482(v),381(v),340(v)
                                                    1472(v),1138(v)
172. CR (   1) B  14                 1.99760    -6.32246  1485(v),1453(v),1475(v)
                                                    1456(v),1472(v),422(v)
                                                    1484(g),1455(g),352(v)
173. CR (   1) B  15                 1.99700    -6.31239  1453(v),1476(v),1488(v)
                                                    408(v),1455(v),1484(g)
                                                    1486(v),226(v),436(v)
                                                    1456(g)
174. CR (   1) C  16                 1.99876    -9.80772  1485(g),1484(v),1496(v)
                                                    1490(v),423(v),1489(v)
                                                    1494(v),452(v)
175. CR (   1) N  17                 1.99942   -13.87266  439(v),466(v),506(v),1485(v)
176. CR (   1) C  18                 1.99904    -9.79290  1490(v),479(v),1491(g)
                                                    1495(v),480(v),452(v)
                                                    1486(v),1093(v)
177. CR (   1) C  19                 1.99904    -9.79352  1496(v),465(v),1491(g)
                                                    1493(v),466(v),494(v)
                                                    1488(v),1098(v)
178. CR (   1) N  20                 1.99942   -13.87399  480(v),646(v),1485(v)
179. CR (   1) C  21                 1.99873    -9.77824  1486(v),576(v),1510(v)
                                                    520(v),1490(g),1502(v)
                                                    1489(v),1498(g),1497(g)
                                                    522(v)
180. CR (   1) C  22                 1.99897    -9.73731  508(v),1490(v),1498(v)
                                                    535(v),536(v),1503(v),592(v)
181. CR (   1) C  23                 1.99910    -9.72359  522(v),549(v),1502(v)
                                                    1497(v),1505(v),1114(v)
182. CR (   1) C  24                 1.99920    -9.72917  563(v),535(v),1500(v)
                                                    1508(v)
183. CR (   1) C  25                 1.99909    -9.72703  549(v),578(v),1510(v)
                                                    1498(v),1503(v)
184. CR (   1) C  26                 1.99898    -9.74018  563(v),508(v),1497(v)
                                                    1490(v),619(v),1505(v)
185. CR (   1) C  27                 1.99936    -9.74236  520(v),1081(v),606(v)
                                                    1497(v),1500(v)
186. CR (   1) C  28                 1.99941    -9.72939  591(v),594(v)
187. CR (   1) C  29                 1.99937    -9.75218  576(v),634(v),1498(v)
                                                    1067(v),1508(v)
188. CR (   1) C  30                 1.99942    -9.73519  1244(v),620(v)
189. CR (   1) C  31                 1.99874    -9.78552  1488(v),716(v),660(v)
                                                    1528(v),1536(v),1496(g)
                                                    1494(v),1524(g),1523(g)
190. CR (   1) C  32                 1.99898    -9.74836  648(v),675(v),1524(v)
                                                    1496(v),731(v),1529(v)
191. CR (   1) C  33                 1.99910    -9.73618  689(v),661(v),662(v),1528(v)
                                                    1531(v),1523(v),1129(v)
192. CR (   1) C  34                 1.99920    -9.73970  703(v),675(v),1534(v)
                                                    1526(v)
193. CR (   1) C  35                 1.99910    -9.73523  717(v),689(v),1536(v)
                                                    1529(v),1524(v)
194. CR (   1) C  36                 1.99898    -9.74625  703(v),648(v),1523(v)
                                                    1496(v),759(v),1531(v)
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195. CR (1) C 37	1.99937	-9.75585	660(v),746(v),983(v),1523(v) 1526(v)
196. CR (1) C 38	1.99942	-9.73816	1304(v)
197. CR (1) C 39	1.99936	-9.75047	716(v),774(v),997(v),1524(v) 1534(v)
198. CR (1) C 40	1.99942	-9.73498	1274(v),1284(v)
199. CR (1) C 41	1.99874	-9.77495	1475(v),855(v),1562(v) 1554(v),800(v),799(v) 1478(g),1477(v),856(v) 1560(v)
200. CR (1) C 42	1.99899	-9.73569	1479(v),788(v),1478(v) 815(v),870(v),1555(v),814(v)
201. CR (1) C 43	1.99911	-9.72450	800(v),828(v),1554(v) 1557(v),1154(v)
202. CR (1) C 44	1.99920	-9.73076	842(v),815(v),1552(v) 1560(v)
203. CR (1) C 45	1.99909	-9.72741	856(v),828(v),1562(v) 1555(v)
204. CR (1) C 46	1.99898	-9.73887	1479(v),842(v),788(v) 1478(v),898(v),1557(v)
205. CR (1) C 47	1.99935	-9.73187	799(v),1011(v),885(v) 1552(v),1549(v)
206. CR (1) C 48	1.99941	-9.72099	871(v)
207. CR (1) C 49	1.99936	-9.74888	855(v),1025(v),913(v) 1550(v),1560(v)
208. CR (1) C 50	1.99942	-9.73323	1424(v)
209. CR (1) C 51	1.99937	-9.74930	282(v),941(v),1461(v) 1039(v),1464(v)
210. CR (1) C 52	1.99942	-9.73320	927(v),1349(v)
211. CR (1) C 53	1.99935	-9.73246	254(v),1053(v),969(v) 1457(v),1458(v)
212. CR (1) C 54	1.99941	-9.72175	955(v)
213. CR (1) C 55	1.99941	-9.72849	732(v)
214. CR (1) C 56	1.99942	-9.72098	760(v)
215. CR (1) C 57	1.99943	-9.71204	870(v)
216. CR (1) C 58	1.99942	-9.72714	899(v),1444(v)
217. CR (1) C 59	1.99941	-9.72782	1335(v),927(v)
218. CR (1) C 60	1.99943	-9.70843	954(v),1384(v)
219. CR (1) C 61	1.99942	-9.72630	620(v),1264(v)
220. CR (1) C 62	1.99942	-9.71137	
221. LP (1) O 2	1.96474	-0.57212	226(v),1456(v),1455(v) 232(v)
222. LP (2) O 2	1.74913	-0.15921	1455(v),1456(v),228(v) 230(v),1565(r)
223. LP*(1) B 14	0.58308	0.02866	224(v),1454(v),1551(r) 1472(v),1475(v),1462(r) 410(g),1484(g),1487(r) 417(g),1455(g)
224. LP (1) B 15	0.74839	0.02727	223(v),1454(v),1487(v) 1488(v),424(g),1486(v) 227(v),1551(r)
225. LP (1) N 20	1.53944	-0.24744	1487(v),1492(v),1523(v) 1524(v),478(v),648(v),441(v)
226. RY*(1) C 1	0.01705	1.01327	
227. RY*(2) C 1	0.00521	2.06636	
228. RY*(3) C 1	0.00290	2.24678	
229. RY*(4) C 1	0.00155	1.76412	
230. RY*(5) C 1	0.00086	0.89622	
231. RY*(6) C 1	0.00055	0.58366	
232. RY*(7) C 1	0.00041	2.40922	
233. RY*(8) C 1	0.00029	1.94890	
234. RY*(9) C 1	0.00015	1.75990	
235. RY*(10) C 1	0.00010	2.24307	
236. RY*(11) C 1	0.00008	1.69330	
237. RY*(12) C 1	0.00002	2.46793	
238. RY*(13) C 1	0.00002	2.63134	
239. RY*(14) C 1	0.00000	20.01219	
240. RY*(1) O 2	0.00533	0.85683	
241. RY*(2) O 2	0.00361	0.78659	
242. RY*(3) O 2	0.00179	1.25683	
243. RY*(4) O 2	0.00041	0.71755	

244.	RY*(5)	O	2	0.00004	4.31106
245.	RY*(6)	O	2	0.00001	2.95893
246.	RY*(7)	O	2	0.00001	3.38809
247.	RY*(8)	O	2	0.00001	2.98594
248.	RY*(9)	O	2	0.00001	4.12688
249.	RY*(10)	O	2	0.00001	2.69385
250.	RY*(11)	O	2	0.00001	2.93138
251.	RY*(12)	O	2	0.00001	3.19118
252.	RY*(13)	O	2	0.00001	2.73098
253.	RY*(14)	O	2	0.00000	41.02280
254.	RY*(1)	C	3	0.00513	1.36040
255.	RY*(2)	C	3	0.00305	1.08649
256.	RY*(3)	C	3	0.00254	0.79294
257.	RY*(4)	C	3	0.00148	1.03935
258.	RY*(5)	C	3	0.00077	1.74847
259.	RY*(6)	C	3	0.00043	1.60159
260.	RY*(7)	C	3	0.00040	1.93876
261.	RY*(8)	C	3	0.00036	2.01019
262.	RY*(9)	C	3	0.00024	1.93989
263.	RY*(10)	C	3	0.00014	2.33322
264.	RY*(11)	C	3	0.00012	2.35496
265.	RY*(12)	C	3	0.00008	1.52046
266.	RY*(13)	C	3	0.00004	2.39600
267.	RY*(14)	C	3	0.00000	21.26725
268.	RY*(1)	C	4	0.00649	1.35795
269.	RY*(2)	C	4	0.00335	0.75199
270.	RY*(3)	C	4	0.00249	1.13961
271.	RY*(4)	C	4	0.00113	1.45530
272.	RY*(5)	C	4	0.00080	1.91383
273.	RY*(6)	C	4	0.00069	2.00971
274.	RY*(7)	C	4	0.00058	1.92933
275.	RY*(8)	C	4	0.00041	1.71307
276.	RY*(9)	C	4	0.00038	1.69483
277.	RY*(10)	C	4	0.00033	1.82971
278.	RY*(11)	C	4	0.00012	2.47991
279.	RY*(12)	C	4	0.00010	2.01067
280.	RY*(13)	C	4	0.00005	2.38717
281.	RY*(14)	C	4	0.00000	21.50815
282.	RY*(1)	C	5	0.00510	1.40435
283.	RY*(2)	C	5	0.00298	0.96586
284.	RY*(3)	C	5	0.00284	0.89740
285.	RY*(4)	C	5	0.00148	1.02311
286.	RY*(5)	C	5	0.00067	1.89250
287.	RY*(6)	C	5	0.00049	1.78158
288.	RY*(7)	C	5	0.00041	1.74489
289.	RY*(8)	C	5	0.00028	1.87015
290.	RY*(9)	C	5	0.00021	1.88335
291.	RY*(10)	C	5	0.00013	2.42101
292.	RY*(11)	C	5	0.00011	2.17567
293.	RY*(12)	C	5	0.00007	1.57664
294.	RY*(13)	C	5	0.00004	2.42354
295.	RY*(14)	C	5	0.00000	21.08030
296.	RY*(1)	C	6	0.00409	1.42571
297.	RY*(2)	C	6	0.00143	1.10791
298.	RY*(3)	C	6	0.00131	0.54220
299.	RY*(4)	C	6	0.00060	1.32875
300.	RY*(5)	C	6	0.00048	1.87643
301.	RY*(6)	C	6	0.00015	2.46131
302.	RY*(7)	C	6	0.00009	1.75899
303.	RY*(8)	C	6	0.00005	2.02057
304.	RY*(9)	C	6	0.00006	1.64486
305.	RY*(10)	C	6	0.00006	1.17888
306.	RY*(11)	C	6	0.00002	1.82149
307.	RY*(12)	C	6	0.00001	1.83985
308.	RY*(13)	C	6	0.00002	2.28675
309.	RY*(14)	C	6	0.00000	20.82809
310.	RY*(1)	C	7	0.00412	1.20618
311.	RY*(2)	C	7	0.00185	1.20728
312.	RY*(3)	C	7	0.00091	0.54798
313.	RY*(4)	C	7	0.00054	1.64307
314.	RY*(5)	C	7	0.00051	1.44725

315.	RY*(	6)	C	7	0.00020	2.41899
316.	RY*(	7)	C	7	0.00007	1.81944
317.	RY*(	8)	C	7	0.00004	2.08090
318.	RY*(	9)	C	7	0.00005	1.47214
319.	RY*(	10)	C	7	0.00004	1.49263
320.	RY*(	11)	C	7	0.00001	1.38395
321.	RY*(	12)	C	7	0.00000	2.13415
322.	RY*(	13)	C	7	0.00000	1.81797
323.	RY*(	14)	C	7	0.00000	21.13564
324.	RY*(	1)	C	8	0.00422	1.41034
325.	RY*(	2)	C	8	0.00147	0.98907
326.	RY*(	3)	C	8	0.00131	0.72525
327.	RY*(	4)	C	8	0.00060	1.31926
328.	RY*(	5)	C	8	0.00046	1.88926
329.	RY*(	6)	C	8	0.00016	2.15460
330.	RY*(	7)	C	8	0.00012	1.77243
331.	RY*(	8)	C	8	0.00008	1.73219
332.	RY*(	9)	C	8	0.00005	2.14760
333.	RY*(	10)	C	8	0.00004	1.49875
334.	RY*(	11)	C	8	0.00002	2.34700
335.	RY*(	12)	C	8	0.00002	1.83220
336.	RY*(	13)	C	8	0.00002	1.70876
337.	RY*(	14)	C	8	0.00000	20.85969
338.	RY*(	1)	N	9	0.00631	0.86041
339.	RY*(	2)	N	9	0.00502	1.39271
340.	RY*(	3)	N	9	0.00155	1.06823
341.	RY*(	4)	N	9	0.00096	1.37893
342.	RY*(	5)	N	9	0.00073	2.23895
343.	RY*(	6)	N	9	0.00052	2.46144
344.	RY*(	7)	N	9	0.00038	2.39264
345.	RY*(	8)	N	9	0.00016	2.51538
346.	RY*(	9)	N	9	0.00013	2.96253
347.	RY*(	10)	N	9	0.00008	3.06821
348.	RY*(	11)	N	9	0.00006	2.84377
349.	RY*(	12)	N	9	0.00004	2.77372
350.	RY*(	13)	N	9	0.00004	2.67353
351.	RY*(	14)	N	9	0.00000	30.12368
352.	RY*(	1)	C	10	0.00546	1.64437
353.	RY*(	2)	C	10	0.00341	1.46986
354.	RY*(	3)	C	10	0.00210	1.67650
355.	RY*(	4)	C	10	0.00162	1.58877
356.	RY*(	5)	C	10	0.00138	1.07496
357.	RY*(	6)	C	10	0.00126	1.41495
358.	RY*(	7)	C	10	0.00112	1.91258
359.	RY*(	8)	C	10	0.00064	1.57027
360.	RY*(	9)	C	10	0.00036	2.96382
361.	RY*(	10)	C	10	0.00014	2.25814
362.	RY*(	11)	C	10	0.00014	2.43904
363.	RY*(	12)	C	10	0.00008	1.90022
364.	RY*(	13)	C	10	0.00004	2.54912
365.	RY*(	14)	C	10	0.00001	20.14700
366.	RY*(	1)	N	11	0.00639	0.80441
367.	RY*(	2)	N	11	0.00514	1.44081
368.	RY*(	3)	N	11	0.00167	1.08092
369.	RY*(	4)	N	11	0.00107	1.09744
370.	RY*(	5)	N	11	0.00067	2.28666
371.	RY*(	6)	N	11	0.00051	2.42712
372.	RY*(	7)	N	11	0.00037	2.41100
373.	RY*(	8)	N	11	0.00015	3.36672
374.	RY*(	9)	N	11	0.00014	2.54294
375.	RY*(	10)	N	11	0.00010	2.71865
376.	RY*(	11)	N	11	0.00006	2.79803
377.	RY*(	12)	N	11	0.00004	2.59223
378.	RY*(	13)	N	11	0.00005	2.76682
379.	RY*(	14)	N	11	0.00000	30.34989
380.	RY*(	1)	C	12	0.00425	0.66917
381.	RY*(	2)	C	12	0.00301	1.33649
382.	RY*(	3)	C	12	0.00144	1.07033
383.	RY*(	4)	C	12	0.00111	1.20621
384.	RY*(	5)	C	12	0.00070	1.76804
385.	RY*(	6)	C	12	0.00041	1.51222

386.	RY*(| 7)	C	12	0.00027	1.51459
387.	RY*(| 8)	C	12	0.00016	1.58051
388.	RY*(| 9)	C	12	0.00011	2.77443
389.	RY*(| 10)	C	12	0.00012	1.87647
390.	RY*(| 11)	C	12	0.00004	1.94999
391.	RY*(| 12)	C	12	0.00002	2.15396
392.	RY*(| 13)	C	12	0.00002	2.22549
393.	RY*(| 14)	C	12	0.00000	21.15827
394.	RY*(| 1)	C	13	0.00426	0.66640
395.	RY*(| 2)	C	13	0.00304	1.32755
396.	RY*(| 3)	C	13	0.00151	1.06108
397.	RY*(| 4)	C	13	0.00109	1.13615
398.	RY*(| 5)	C	13	0.00069	1.77057
399.	RY*(| 6)	C	13	0.00044	1.52489
400.	RY*(| 7)	C	13	0.00024	1.59842
401.	RY*(| 8)	C	13	0.00015	1.54848
402.	RY*(| 9)	C	13	0.00012	1.83921
403.	RY*(| 10)	C	13	0.00009	2.68318
404.	RY*(| 11)	C	13	0.00005	1.96632
405.	RY*(| 12)	C	13	0.00002	2.36807
406.	RY*(| 13)	C	13	0.00002	1.96302
407.	RY*(| 14)	C	13	0.00000	21.20581
408.	RY*(| 1)	B	14	0.00292	1.51642
409.	RY*(| 2)	B	14	0.00140	1.12391
410.	RY*(| 3)	B	14	0.00130	0.68131
411.	RY*(| 4)	B	14	0.00095	1.21312
412.	RY*(| 5)	B	14	0.00063	1.82633
413.	RY*(| 6)	B	14	0.00045	3.45858
414.	RY*(| 7)	B	14	0.00038	2.53228
415.	RY*(| 8)	B	14	0.00037	1.32806
416.	RY*(| 9)	B	14	0.00019	4.46769
417.	RY*(| 10)	B	14	0.00013	1.73210
418.	RY*(| 11)	B	14	0.00009	2.40818
419.	RY*(| 12)	B	14	0.00007	4.17733
420.	RY*(| 13)	B	14	0.00004	2.80608
421.	RY*(| 14)	B	14	0.00004	1.46847
422.	RY*(| 1)	B	15	0.00328	1.63071
423.	RY*(| 2)	B	15	0.00182	1.36655
424.	RY*(| 3)	B	15	0.00127	0.81808
425.	RY*(| 4)	B	15	0.00122	0.88663
426.	RY*(| 5)	B	15	0.00116	1.23454
427.	RY*(| 6)	B	15	0.00070	1.60540
428.	RY*(| 7)	B	15	0.00037	1.85419
429.	RY*(| 8)	B	15	0.00028	1.91498
430.	RY*(| 9)	B	15	0.00024	6.45575
431.	RY*(| 10)	B	15	0.00017	1.37163
432.	RY*(| 11)	B	15	0.00009	3.05138
433.	RY*(| 12)	B	15	0.00006	3.97689
434.	RY*(| 13)	B	15	0.00005	2.21913
435.	RY*(| 14)	B	15	0.00003	1.54081
436.	RY*(| 1)	C	16	0.00549	1.82074
437.	RY*(| 2)	C	16	0.00277	1.24577
438.	RY*(| 3)	C	16	0.00260	1.44969
439.	RY*(| 4)	C	16	0.00186	1.51680
440.	RY*(| 5)	C	16	0.00133	1.53010
441.	RY*(| 6)	C	16	0.00128	1.64433
442.	RY*(| 7)	C	16	0.00081	1.54722
443.	RY*(| 8)	C	16	0.00077	1.62727
444.	RY*(| 9)	C	16	0.00044	2.66454
445.	RY*(| 10)	C	16	0.00019	2.28912
446.	RY*(| 11)	C	16	0.00013	2.38826
447.	RY*(| 12)	C	16	0.00008	1.77313
448.	RY*(| 13)	C	16	0.00004	2.49186
449.	RY*(| 14)	C	16	0.00001	20.13101
450.	RY*(| 1)	N	17	0.00554	1.47691
451.	RY*(| 2)	N	17	0.00483	0.74416
452.	RY*(| 3)	N	17	0.00166	0.95593
453.	RY*(| 4)	N	17	0.00121	1.05250
454.	RY*(| 5)	N	17	0.00075	2.26074
455.	RY*(| 6)	N	17	0.00065	2.54354
456.	RY*(| 7)	N	17	0.00032	2.42112

457.	RY*(| 8)	N	17	0.00014	2.57254
458.	RY*(| 9)	N	17	0.00014	3.66045
459.	RY*(| 10)	N	17	0.00010	2.39969
460.	RY*(| 11)	N	17	0.00005	2.74666
461.	RY*(| 12)	N	17	0.00005	2.77887
462.	RY*(| 13)	N	17	0.00004	2.58033
463.	RY*(| 14)	N	17	0.00000	30.33750
464.	RY*(| 1)	C	18	0.00366	0.62106
465.	RY*(| 2)	C	18	0.00314	1.33367
466.	RY*(| 3)	C	18	0.00146	1.11204
467.	RY*(| 4)	C	18	0.00107	1.16292
468.	RY*(| 5)	C	18	0.00069	1.73324
469.	RY*(| 6)	C	18	0.00044	1.51841
470.	RY*(| 7)	C	18	0.00024	1.50709
471.	RY*(| 8)	C	18	0.00016	1.55830
472.	RY*(| 9)	C	18	0.00011	2.78261
473.	RY*(| 10)	C	18	0.00009	1.93399
474.	RY*(| 11)	C	18	0.00002	2.32009
475.	RY*(| 12)	C	18	0.00003	1.96348
476.	RY*(| 13)	C	18	0.00003	1.78847
477.	RY*(| 14)	C	18	0.00000	21.19451
478.	RY*(| 1)	C	19	0.00371	0.60162
479.	RY*(| 2)	C	19	0.00308	1.28984
480.	RY*(| 3)	C	19	0.00145	1.09088
481.	RY*(| 4)	C	19	0.00096	1.13833
482.	RY*(| 5)	C	19	0.00064	1.74045
483.	RY*(| 6)	C	19	0.00048	1.49431
484.	RY*(| 7)	C	19	0.00025	1.43770
485.	RY*(| 8)	C	19	0.00014	1.44889
486.	RY*(| 9)	C	19	0.00011	2.66697
487.	RY*(| 10)	C	19	0.00010	1.96083
488.	RY*(| 11)	C	19	0.00005	1.85238
489.	RY*(| 12)	C	19	0.00002	2.31332
490.	RY*(| 13)	C	19	0.00003	1.91607
491.	RY*(| 14)	C	19	0.00000	21.26988
492.	RY*(| 1)	N	20	0.00571	1.38800
493.	RY*(| 2)	N	20	0.00498	0.83845
494.	RY*(| 3)	N	20	0.00169	1.03314
495.	RY*(| 4)	N	20	0.00108	1.07873
496.	RY*(| 5)	N	20	0.00071	2.23723
497.	RY*(| 6)	N	20	0.00059	2.46686
498.	RY*(| 7)	N	20	0.00032	2.39518
499.	RY*(| 8)	N	20	0.00014	3.73019
500.	RY*(| 9)	N	20	0.00015	2.57253
501.	RY*(| 10)	N	20	0.00009	2.39176
502.	RY*(| 11)	N	20	0.00006	2.66734
503.	RY*(| 12)	N	20	0.00004	2.55714
504.	RY*(| 13)	N	20	0.00004	2.81008
505.	RY*(| 14)	N	20	0.00000	30.32997
506.	RY*(| 1)	C	21	0.00680	1.26166
507.	RY*(| 2)	C	21	0.00357	0.75510
508.	RY*(| 3)	C	21	0.00291	0.98383
509.	RY*(| 4)	C	21	0.00116	1.65958
510.	RY*(| 5)	C	21	0.00089	1.97133
511.	RY*(| 6)	C	21	0.00078	2.03284
512.	RY*(| 7)	C	21	0.00068	1.79172
513.	RY*(| 8)	C	21	0.00043	1.67201
514.	RY*(| 9)	C	21	0.00039	1.91834
515.	RY*(| 10)	C	21	0.00036	1.73677
516.	RY*(| 11)	C	21	0.00014	2.47545
517.	RY*(| 12)	C	21	0.00010	2.03250
518.	RY*(| 13)	C	21	0.00005	2.39117
519.	RY*(| 14)	C	21	0.00000	21.08259
520.	RY*(| 1)	C	22	0.00535	1.29617
521.	RY*(| 2)	C	22	0.00398	0.68533
522.	RY*(| 3)	C	22	0.00332	0.96731
523.	RY*(| 4)	C	22	0.00190	1.05795
524.	RY*(| 5)	C	22	0.00075	1.77380
525.	RY*(| 6)	C	22	0.00047	1.69043
526.	RY*(| 7)	C	22	0.00045	1.93423
527.	RY*(| 8)	C	22	0.00033	1.89721

528.	RY*(9)	C	22	0.00028	1.93297
529.	RY*(10)	C	22	0.00014	2.35530
530.	RY*(11)	C	22	0.00013	2.44804
531.	RY*(12)	C	22	0.00008	1.64291
532.	RY*(13)	C	22	0.00004	2.37242
533.	RY*(14)	C	22	0.00000	21.05229
534.	RY*(1)	C	23	0.00409	1.43011
535.	RY*(2)	C	23	0.00148	0.85360
536.	RY*(3)	C	23	0.00141	0.84501
537.	RY*(4)	C	23	0.00067	1.33279
538.	RY*(5)	C	23	0.00046	1.86317
539.	RY*(6)	C	23	0.00015	2.09906
540.	RY*(7)	C	23	0.00011	1.89271
541.	RY*(8)	C	23	0.00009	1.63100
542.	RY*(9)	C	23	0.00005	2.09029
543.	RY*(10)	C	23	0.00003	1.47780
544.	RY*(11)	C	23	0.00003	1.64945
545.	RY*(12)	C	23	0.00002	1.89749
546.	RY*(13)	C	23	0.00002	2.36283
547.	RY*(14)	C	23	0.00000	20.72293
548.	RY*(1)	C	24	0.00400	1.21961
549.	RY*(2)	C	24	0.00185	1.20740
550.	RY*(3)	C	24	0.00092	0.57985
551.	RY*(4)	C	24	0.00055	1.28574
552.	RY*(5)	C	24	0.00048	1.75343
553.	RY*(6)	C	24	0.00020	2.39821
554.	RY*(7)	C	24	0.00007	1.72726
555.	RY*(8)	C	24	0.00005	1.56898
556.	RY*(9)	C	24	0.00004	2.45717
557.	RY*(10)	C	24	0.00004	1.05800
558.	RY*(11)	C	24	0.00001	1.63880
559.	RY*(12)	C	24	0.00000	20.98464
560.	RY*(13)	C	24	0.00001	1.82882
561.	RY*(14)	C	24	0.00000	2.06682
562.	RY*(1)	C	25	0.00401	1.42687
563.	RY*(2)	C	25	0.00145	1.09920
564.	RY*(3)	C	25	0.00127	0.57105
565.	RY*(4)	C	25	0.00061	1.37236
566.	RY*(5)	C	25	0.00048	1.86278
567.	RY*(6)	C	25	0.00015	2.45316
568.	RY*(7)	C	25	0.00008	1.84181
569.	RY*(8)	C	25	0.00006	1.33264
570.	RY*(9)	C	25	0.00005	1.60813
571.	RY*(10)	C	25	0.00005	2.02944
572.	RY*(11)	C	25	0.00002	2.07874
573.	RY*(12)	C	25	0.00001	1.95048
574.	RY*(13)	C	25	0.00002	1.68958
575.	RY*(14)	C	25	0.00000	20.89797
576.	RY*(1)	C	26	0.00511	1.40275
577.	RY*(2)	C	26	0.00300	0.79518
578.	RY*(3)	C	26	0.00288	1.06032
579.	RY*(4)	C	26	0.00144	1.09941
580.	RY*(5)	C	26	0.00075	1.82876
581.	RY*(6)	C	26	0.00052	1.82635
582.	RY*(7)	C	26	0.00044	1.72988
583.	RY*(8)	C	26	0.00028	1.88543
584.	RY*(9)	C	26	0.00020	1.96859
585.	RY*(10)	C	26	0.00013	2.37367
586.	RY*(11)	C	26	0.00011	2.03416
587.	RY*(12)	C	26	0.00009	1.71604
588.	RY*(13)	C	26	0.00004	2.40133
589.	RY*(14)	C	26	0.00000	21.21474
590.	RY*(1)	C	27	0.00369	1.07451
591.	RY*(2)	C	27	0.00170	1.01853
592.	RY*(3)	C	27	0.00140	1.50695
593.	RY*(4)	C	27	0.00074	1.45826
594.	RY*(5)	C	27	0.00059	1.45970
595.	RY*(6)	C	27	0.00037	1.62695
596.	RY*(7)	C	27	0.00029	1.94461
597.	RY*(8)	C	27	0.00025	1.97490
598.	RY*(9)	C	27	0.00019	1.84562

599.	RY*(| 10)	C	27	0.00016	2.20042
600.	RY*(| 11)	C	27	0.00011	1.99794
601.	RY*(| 12)	C	27	0.00008	1.83850
602.	RY*(| 13)	C	27	0.00003	2.35516
603.	RY*(| 14)	C	27	0.00000	20.73567
604.	RY*(| 1)	C	28	0.00154	0.87861
605.	RY*(| 2)	C	28	0.00098	0.88762
606.	RY*(| 3)	C	28	0.00025	1.13357
607.	RY*(| 4)	C	28	0.00014	1.47420
608.	RY*(| 5)	C	28	0.00011	1.99043
609.	RY*(| 6)	C	28	0.00008	1.42522
610.	RY*(| 7)	C	28	0.00004	1.95821
611.	RY*(| 8)	C	28	0.00003	1.48670
612.	RY*(| 9)	C	28	0.00001	2.20505
613.	RY*(| 10)	C	28	0.00001	2.27083
614.	RY*(| 11)	C	28	0.00001	1.93263
615.	RY*(| 12)	C	28	0.00001	1.99471
616.	RY*(| 13)	C	28	0.00000	20.19853
617.	RY*(| 14)	C	28	0.00001	2.23411
618.	RY*(| 1)	C	29	0.00356	1.11446
619.	RY*(| 2)	C	29	0.00128	1.56719
620.	RY*(| 3)	C	29	0.00112	1.03211
621.	RY*(| 4)	C	29	0.00066	1.85552
622.	RY*(| 5)	C	29	0.00050	1.68925
623.	RY*(| 6)	C	29	0.00032	1.19988
624.	RY*(| 7)	C	29	0.00025	1.74781
625.	RY*(| 8)	C	29	0.00026	1.99054
626.	RY*(| 9)	C	29	0.00017	2.04295
627.	RY*(| 10)	C	29	0.00014	1.85387
628.	RY*(| 11)	C	29	0.00010	2.01242
629.	RY*(| 12)	C	29	0.00002	1.69866
630.	RY*(| 13)	C	29	0.00002	2.37057
631.	RY*(| 14)	C	29	0.00000	21.06842
632.	RY*(| 1)	C	30	0.00169	0.78371
633.	RY*(| 2)	C	30	0.00101	0.81884
634.	RY*(| 3)	C	30	0.00032	1.02937
635.	RY*(| 4)	C	30	0.00017	1.65150
636.	RY*(| 5)	C	30	0.00010	1.82214
637.	RY*(| 6)	C	30	0.00007	1.12063
638.	RY*(| 7)	C	30	0.00003	2.19296
639.	RY*(| 8)	C	30	0.00003	2.18010
640.	RY*(| 9)	C	30	0.00001	2.13537
641.	RY*(| 10)	C	30	0.00001	1.58624
642.	RY*(| 11)	C	30	0.00001	2.25757
643.	RY*(| 12)	C	30	0.00001	2.06048
644.	RY*(| 13)	C	30	0.00001	2.26927
645.	RY*(| 14)	C	30	0.00000	19.89249
646.	RY*(| 1)	C	31	0.00656	1.31066
647.	RY*(| 2)	C	31	0.00339	0.74244
648.	RY*(| 3)	C	31	0.00263	1.09453
649.	RY*(| 4)	C	31	0.00107	1.60023
650.	RY*(| 5)	C	31	0.00083	1.88736
651.	RY*(| 6)	C	31	0.00075	1.82147
652.	RY*(| 7)	C	31	0.00059	1.90762
653.	RY*(| 8)	C	31	0.00044	1.64648
654.	RY*(| 9)	C	31	0.00035	1.95656
655.	RY*(| 10)	C	31	0.00029	1.50728
656.	RY*(| 11)	C	31	0.00012	2.10127
657.	RY*(| 12)	C	31	0.00013	2.42316
658.	RY*(| 13)	C	31	0.00005	2.37701
659.	RY*(| 14)	C	31	0.00000	21.52271
660.	RY*(| 1)	C	32	0.00502	1.40023
661.	RY*(| 2)	C	32	0.00294	0.92683
662.	RY*(| 3)	C	32	0.00278	0.87766
663.	RY*(| 4)	C	32	0.00147	1.00288
664.	RY*(| 5)	C	32	0.00065	1.85859
665.	RY*(| 6)	C	32	0.00051	1.58302
666.	RY*(| 7)	C	32	0.00049	1.83714
667.	RY*(| 8)	C	32	0.00028	1.84133
668.	RY*(| 9)	C	32	0.00021	1.90270
669.	RY*(| 10)	C	32	0.00015	2.23087

670.	RY*(	11)	C	32	0.00012 2.32600
671.	RY*(	12)	C	32	0.00007 1.62840
672.	RY*(	13)	C	32	0.00004 2.43843
673.	RY*(	14)	C	32	0.00000 21.02273
674.	RY*(	1)	C	33	0.00405 1.42094
675.	RY*(	2)	C	33	0.00148 0.92574
676.	RY*(	3)	C	33	0.00134 0.73533
677.	RY*(	4)	C	33	0.00059 1.30583
678.	RY*(	5)	C	33	0.00046 1.84583
679.	RY*(	6)	C	33	0.00015 2.35714
680.	RY*(	7)	C	33	0.00009 1.60427
681.	RY*(	8)	C	33	0.00008 1.76578
682.	RY*(	9)	C	33	0.00005 2.02875
683.	RY*(	10)	C	33	0.00004 1.29388
684.	RY*(	11)	C	33	0.00003 2.02721
685.	RY*(	12)	C	33	0.00002 1.77069
686.	RY*(	13)	C	33	0.00001 2.25693
687.	RY*(	14)	C	33	0.00000 20.72953
688.	RY*(	1)	C	34	0.00413 1.20527
689.	RY*(	2)	C	34	0.00186 1.19862
690.	RY*(	3)	C	34	0.00087 0.60028
691.	RY*(	4)	C	34	0.00054 1.21976
692.	RY*(	5)	C	34	0.00052 1.81578
693.	RY*(	6)	C	34	0.00019 2.48350
694.	RY*(	7)	C	34	0.00007 1.75117
695.	RY*(	8)	C	34	0.00005 1.56793
696.	RY*(	9)	C	34	0.00003 1.20830
697.	RY*(	10)	C	34	0.00003 2.32334
698.	RY*(	11)	C	34	0.00003 1.34390
699.	RY*(	12)	C	34	0.00000 21.19523
700.	RY*(	13)	C	34	0.00000 2.11279
701.	RY*(	14)	C	34	0.00001 1.84082
702.	RY*(	1)	C	35	0.00425 1.39464
703.	RY*(	2)	C	35	0.00143 1.08223
704.	RY*(	3)	C	35	0.00118 0.58165
705.	RY*(	4)	C	35	0.00061 1.33642
706.	RY*(	5)	C	35	0.00048 1.89269
707.	RY*(	6)	C	35	0.00015 2.36928
708.	RY*(	7)	C	35	0.00009 1.53356
709.	RY*(	8)	C	35	0.00009 1.81178
710.	RY*(	9)	C	35	0.00007 1.69662
711.	RY*(	10)	C	35	0.00004 1.81889
712.	RY*(	11)	C	35	0.00002 2.39680
713.	RY*(	12)	C	35	0.00002 1.71308
714.	RY*(	13)	C	35	0.00002 1.75749
715.	RY*(	14)	C	35	0.00000 20.97916
716.	RY*(	1)	C	36	0.00522 1.38785
717.	RY*(	2)	C	36	0.00289 1.11489
718.	RY*(	3)	C	36	0.00273 0.78591
719.	RY*(	4)	C	36	0.00147 1.00443
720.	RY*(	5)	C	36	0.00078 1.72002
721.	RY*(	6)	C	36	0.00050 1.86882
722.	RY*(	7)	C	36	0.00044 1.76751
723.	RY*(	8)	C	36	0.00027 1.83754
724.	RY*(	9)	C	36	0.00020 1.96710
725.	RY*(	10)	C	36	0.00011 2.23224
726.	RY*(	11)	C	36	0.00012 2.38816
727.	RY*(	12)	C	36	0.00007 1.50722
728.	RY*(	13)	C	36	0.00004 2.41555
729.	RY*(	14)	C	36	0.00000 21.10423
730.	RY*(	1)	C	37	0.00347 1.11172
731.	RY*(	2)	C	37	0.00128 1.55433
732.	RY*(	3)	C	37	0.00115 1.04105
733.	RY*(	4)	C	37	0.00063 1.85777
734.	RY*(	5)	C	37	0.00052 1.61670
735.	RY*(	6)	C	37	0.00034 1.34701
736.	RY*(	7)	C	37	0.00026 2.03953
737.	RY*(	8)	C	37	0.00024 1.69003
738.	RY*(	9)	C	37	0.00017 2.09726
739.	RY*(	10)	C	37	0.00014 1.54559
740.	RY*(	11)	C	37	0.00011 2.21133

741.	RY*(12)	C	37	0.00002	2.34541
742.	RY*(13)	C	37	0.00002	1.60226
743.	RY*(14)	C	37	0.00000	21.05146
744.	RY*(1)	C	38	0.00174	0.76422
745.	RY*(2)	C	38	0.00102	0.79899
746.	RY*(3)	C	38	0.00031	1.04405
747.	RY*(4)	C	38	0.00018	1.63725
748.	RY*(5)	C	38	0.00009	2.10488
749.	RY*(6)	C	38	0.00007	1.07652
750.	RY*(7)	C	38	0.00003	2.03099
751.	RY*(8)	C	38	0.00003	2.21275
752.	RY*(9)	C	38	0.00001	2.17802
753.	RY*(10)	C	38	0.00000	2.14706
754.	RY*(11)	C	38	0.00001	1.44735
755.	RY*(12)	C	38	0.00000	20.03623
756.	RY*(13)	C	38	0.00001	2.12395
757.	RY*(14)	C	38	0.00001	2.17525
758.	RY*(1)	C	39	0.00358	1.11088
759.	RY*(2)	C	39	0.00126	1.56478
760.	RY*(3)	C	39	0.00115	1.10332
761.	RY*(4)	C	39	0.00064	1.82355
762.	RY*(5)	C	39	0.00052	1.61346
763.	RY*(6)	C	39	0.00031	1.38491
764.	RY*(7)	C	39	0.00026	1.90043
765.	RY*(8)	C	39	0.00021	1.75763
766.	RY*(9)	C	39	0.00017	1.77728
767.	RY*(10)	C	39	0.00014	1.94923
768.	RY*(11)	C	39	0.00010	2.13538
769.	RY*(12)	C	39	0.00002	2.36335
770.	RY*(13)	C	39	0.00002	1.72160
771.	RY*(14)	C	39	0.00000	21.10891
772.	RY*(1)	C	40	0.00162	0.80115
773.	RY*(2)	C	40	0.00097	0.86810
774.	RY*(3)	C	40	0.00029	1.09501
775.	RY*(4)	C	40	0.00015	1.57837
776.	RY*(5)	C	40	0.00010	1.90747
777.	RY*(6)	C	40	0.00007	1.07427
778.	RY*(7)	C	40	0.00002	2.39826
779.	RY*(8)	C	40	0.00002	2.16151
780.	RY*(9)	C	40	0.00003	1.83712
781.	RY*(10)	C	40	0.00001	1.91058
782.	RY*(11)	C	40	0.00001	2.28483
783.	RY*(12)	C	40	0.00000	19.75255
784.	RY*(13)	C	40	0.00000	2.05289
785.	RY*(14)	C	40	0.00000	2.07569
786.	RY*(1)	C	41	0.00651	1.29334
787.	RY*(2)	C	41	0.00320	0.78456
788.	RY*(3)	C	41	0.00141	1.46775
789.	RY*(4)	C	41	0.00100	1.60672
790.	RY*(5)	C	41	0.00082	1.73202
791.	RY*(6)	C	41	0.00072	1.85729
792.	RY*(7)	C	41	0.00041	1.59003
793.	RY*(8)	C	41	0.00039	1.60768
794.	RY*(9)	C	41	0.00033	1.79911
795.	RY*(10)	C	41	0.00014	2.52782
796.	RY*(11)	C	41	0.00010	2.00438
797.	RY*(12)	C	41	0.00005	2.42632
798.	RY*(13)	C	41	0.00000	21.49869
799.	RY*(1)	C	42	0.00502	1.37073
800.	RY*(2)	C	42	0.00306	1.05399
801.	RY*(3)	C	42	0.00236	0.83093
802.	RY*(4)	C	42	0.00137	1.01323
803.	RY*(5)	C	42	0.00065	1.79599
804.	RY*(6)	C	42	0.00050	1.66194
805.	RY*(7)	C	42	0.00042	1.84188
806.	RY*(8)	C	42	0.00033	1.94340
807.	RY*(9)	C	42	0.00024	1.86148
808.	RY*(10)	C	42	0.00013	2.39967
809.	RY*(11)	C	42	0.00012	2.32188
810.	RY*(12)	C	42	0.00007	1.49644
811.	RY*(13)	C	42	0.00004	2.40081

812.	RY*(| 14)	C	42	0.00000	21.24455
813.	RY*(| 1)	C	43	0.00409	1.42440
814.	RY*(| 2)	C	43	0.00153	0.74522
815.	RY*(| 3)	C	43	0.00136	0.89835
816.	RY*(| 4)	C	43	0.00060	1.31234
817.	RY*(| 5)	C	43	0.00047	1.89305
818.	RY*(| 6)	C	43	0.00015	2.13339
819.	RY*(| 7)	C	43	0.00012	1.76076
820.	RY*(| 8)	C	43	0.00007	1.72613
821.	RY*(| 9)	C	43	0.00006	1.54950
822.	RY*(| 10)	C	43	0.00005	2.18092
823.	RY*(| 11)	C	43	0.00002	1.60456
824.	RY*(| 12)	C	43	0.00002	2.05788
825.	RY*(| 13)	C	43	0.00002	2.17061
826.	RY*(| 14)	C	43	0.00000	20.69190
827.	RY*(| 1)	C	44	0.00417	1.19292
828.	RY*(| 2)	C	44	0.00187	1.19094
829.	RY*(| 3)	C	44	0.00089	0.57026
830.	RY*(| 4)	C	44	0.00051	1.14427
831.	RY*(| 5)	C	44	0.00051	1.89391
832.	RY*(| 6)	C	44	0.00020	2.41379
833.	RY*(| 7)	C	44	0.00008	1.44881
834.	RY*(| 8)	C	44	0.00007	1.86756
835.	RY*(| 9)	C	44	0.00004	1.10283
836.	RY*(| 10)	C	44	0.00004	2.40962
837.	RY*(| 11)	C	44	0.00001	1.48713
838.	RY*(| 12)	C	44	0.00000	21.10410
839.	RY*(| 13)	C	44	0.00000	1.95213
840.	RY*(| 14)	C	44	0.00000	1.99776
841.	RY*(| 1)	C	45	0.00417	1.41751
842.	RY*(| 2)	C	45	0.00144	1.10804
843.	RY*(| 3)	C	45	0.00134	0.52591
844.	RY*(| 4)	C	45	0.00061	1.31931
845.	RY*(| 5)	C	45	0.00049	1.88409
846.	RY*(| 6)	C	45	0.00015	2.43395
847.	RY*(| 7)	C	45	0.00010	1.72748
848.	RY*(| 8)	C	45	0.00008	1.61927
849.	RY*(| 9)	C	45	0.00005	1.83285
850.	RY*(| 10)	C	45	0.00006	1.47902
851.	RY*(| 11)	C	45	0.00002	1.73710
852.	RY*(| 12)	C	45	0.00002	1.72581
853.	RY*(| 13)	C	45	0.00001	2.52772
854.	RY*(| 14)	C	45	0.00000	20.81206
855.	RY*(| 1)	C	46	0.00513	1.39508
856.	RY*(| 2)	C	46	0.00295	1.13359
857.	RY*(| 3)	C	46	0.00289	0.73772
858.	RY*(| 4)	C	46	0.00146	0.99230
859.	RY*(| 5)	C	46	0.00067	1.84337
860.	RY*(| 6)	C	46	0.00052	1.77018
861.	RY*(| 7)	C	46	0.00049	1.77683
862.	RY*(| 8)	C	46	0.00029	1.85810
863.	RY*(| 9)	C	46	0.00020	1.85277
864.	RY*(| 10)	C	46	0.00012	2.18111
865.	RY*(| 11)	C	46	0.00013	2.45043
866.	RY*(| 12)	C	46	0.00009	1.57850
867.	RY*(| 13)	C	46	0.00004	2.44708
868.	RY*(| 14)	C	46	0.00000	21.14819
869.	RY*(| 1)	C	47	0.00368	1.05182
870.	RY*(| 2)	C	47	0.00178	1.12326
871.	RY*(| 3)	C	47	0.00140	1.07268
872.	RY*(| 4)	C	47	0.00067	1.35637
873.	RY*(| 5)	C	47	0.00059	1.81766
874.	RY*(| 6)	C	47	0.00042	1.61515
875.	RY*(| 7)	C	47	0.00029	2.12143
876.	RY*(| 8)	C	47	0.00030	1.93697
877.	RY*(| 9)	C	47	0.00023	2.00734
878.	RY*(| 10)	C	47	0.00013	2.15006
879.	RY*(| 11)	C	47	0.00011	1.91547
880.	RY*(| 12)	C	47	0.00011	2.10256
881.	RY*(| 13)	C	47	0.00003	2.40793
882.	RY*(| 14)	C	47	0.00000	20.59374

883.	RY*(| 1)	C	48	0.00153	0.89739
884.	RY*(| 2)	C	48	0.00099	0.88917
885.	RY*(| 3)	C	48	0.00029	1.10237
886.	RY*(| 4)	C	48	0.00011	1.53479
887.	RY*(| 5)	C	48	0.00012	1.92114
888.	RY*(| 6)	C	48	0.00007	1.41484
889.	RY*(| 7)	C	48	0.00004	1.82710
890.	RY*(| 8)	C	48	0.00003	1.78266
891.	RY*(| 9)	C	48	0.00002	2.15469
892.	RY*(| 10)	C	48	0.00000	20.26540
893.	RY*(| 11)	C	48	0.00001	2.18503
894.	RY*(| 12)	C	48	0.00001	2.37077
895.	RY*(| 13)	C	48	0.00001	1.87255
896.	RY*(| 14)	C	48	0.00000	1.99554
897.	RY*(| 1)	C	49	0.00367	1.11390
898.	RY*(| 2)	C	49	0.00133	1.50354
899.	RY*(| 3)	C	49	0.00128	0.97614
900.	RY*(| 4)	C	49	0.00068	1.82033
901.	RY*(| 5)	C	49	0.00050	1.71271
902.	RY*(| 6)	C	49	0.00034	1.18764
903.	RY*(| 7)	C	49	0.00026	2.01543
904.	RY*(| 8)	C	49	0.00027	1.85296
905.	RY*(| 9)	C	49	0.00018	2.07750
906.	RY*(| 10)	C	49	0.00015	1.94249
907.	RY*(| 11)	C	49	0.00009	1.93912
908.	RY*(| 12)	C	49	0.00002	2.40316
909.	RY*(| 13)	C	49	0.00003	1.73871
910.	RY*(| 14)	C	49	0.00000	21.05163
911.	RY*(| 1)	C	50	0.00165	0.78947
912.	RY*(| 2)	C	50	0.00104	0.81353
913.	RY*(| 3)	C	50	0.00038	1.03892
914.	RY*(| 4)	C	50	0.00016	1.64499
915.	RY*(| 5)	C	50	0.00011	1.59273
916.	RY*(| 6)	C	50	0.00008	1.35592
917.	RY*(| 7)	C	50	0.00002	2.58044
918.	RY*(| 8)	C	50	0.00003	2.01151
919.	RY*(| 9)	C	50	0.00002	2.21122
920.	RY*(| 10)	C	50	0.00001	1.77478
921.	RY*(| 11)	C	50	0.00000	19.86859
922.	RY*(| 12)	C	50	0.00000	1.96082
923.	RY*(| 13)	C	50	0.00001	2.05054
924.	RY*(| 14)	C	50	0.00001	2.13968
925.	RY*(| 1)	C	51	0.00364	1.11878
926.	RY*(| 2)	C	51	0.00135	1.51456
927.	RY*(| 3)	C	51	0.00123	0.97902
928.	RY*(| 4)	C	51	0.00063	1.87977
929.	RY*(| 5)	C	51	0.00048	1.75478
930.	RY*(| 6)	C	51	0.00035	1.22905
931.	RY*(| 7)	C	51	0.00026	2.02870
932.	RY*(| 8)	C	51	0.00025	1.78002
933.	RY*(| 9)	C	51	0.00018	2.13643
934.	RY*(| 10)	C	51	0.00013	1.77343
935.	RY*(| 11)	C	51	0.00010	2.00360
936.	RY*(| 12)	C	51	0.00003	1.59978
937.	RY*(| 13)	C	51	0.00002	2.40986
938.	RY*(| 14)	C	51	0.00000	20.96727
939.	RY*(| 1)	C	52	0.00168	0.78408
940.	RY*(| 2)	C	52	0.00104	0.79820
941.	RY*(| 3)	C	52	0.00037	1.03305
942.	RY*(| 4)	C	52	0.00017	1.63770
943.	RY*(| 5)	C	52	0.00011	1.76026
944.	RY*(| 6)	C	52	0.00008	1.24998
945.	RY*(| 7)	C	52	0.00002	2.01962
946.	RY*(| 8)	C	52	0.00001	1.49881
947.	RY*(| 9)	C	52	0.00001	2.92172
948.	RY*(| 10)	C	52	0.00001	2.23886
949.	RY*(| 11)	C	52	0.00002	2.28413
950.	RY*(| 12)	C	52	0.00002	1.88797
951.	RY*(| 13)	C	52	0.00000	19.55501
952.	RY*(| 14)	C	52	0.00001	2.18088
953.	RY*(| 1)	C	53	0.00371	1.04881

954.	RY*(| 2)	C	53	0.00163	1.11006
955.	RY*(| 3)	C	53	0.00137	1.18159
956.	RY*(| 4)	C	53	0.00073	1.28911
957.	RY*(| 5)	C	53	0.00061	1.82151
958.	RY*(| 6)	C	53	0.00039	1.61798
959.	RY*(| 7)	C	53	0.00032	1.85403
960.	RY*(| 8)	C	53	0.00029	2.11923
961.	RY*(| 9)	C	53	0.00021	2.09148
962.	RY*(| 10)	C	53	0.00013	2.16627
963.	RY*(| 11)	C	53	0.00010	1.99784
964.	RY*(| 12)	C	53	0.00011	1.95924
965.	RY*(| 13)	C	53	0.00003	2.41283
966.	RY*(| 14)	C	53	0.00000	20.60996
967.	RY*(| 1)	C	54	0.00150	0.88589
968.	RY*(| 2)	C	54	0.00097	0.90000
969.	RY*(| 3)	C	54	0.00026	1.13126
970.	RY*(| 4)	C	54	0.00011	2.06076
971.	RY*(| 5)	C	54	0.00012	1.46467
972.	RY*(| 6)	C	54	0.00007	1.33664
973.	RY*(| 7)	C	54	0.00003	1.95964
974.	RY*(| 8)	C	54	0.00003	1.59809
975.	RY*(| 9)	C	54	0.00003	2.13764
976.	RY*(| 10)	C	54	0.00001	2.26031
977.	RY*(| 11)	C	54	0.00001	1.89090
978.	RY*(| 12)	C	54	0.00000	2.13906
979.	RY*(| 13)	C	54	0.00001	2.09598
980.	RY*(| 14)	C	54	0.00000	20.25877
981.	RY*(| 1)	C	55	0.00160	0.94782
982.	RY*(| 2)	C	55	0.00113	0.97102
983.	RY*(| 3)	C	55	0.00043	0.91350
984.	RY*(| 4)	C	55	0.00016	1.21927
985.	RY*(| 5)	C	55	0.00015	1.74633
986.	RY*(| 6)	C	55	0.00009	1.80177
987.	RY*(| 7)	C	55	0.00009	2.38474
988.	RY*(| 8)	C	55	0.00004	1.53856
989.	RY*(| 9)	C	55	0.00004	2.25705
990.	RY*(| 10)	C	55	0.00001	2.28460
991.	RY*(| 11)	C	55	0.00002	1.87601
992.	RY*(| 12)	C	55	0.00000	20.47851
993.	RY*(| 13)	C	55	0.00001	2.43918
994.	RY*(| 14)	C	55	0.00001	2.36213
995.	RY*(| 1)	C	56	0.00167	0.94447
996.	RY*(| 2)	C	56	0.00111	0.93842
997.	RY*(| 3)	C	56	0.00050	0.85093
998.	RY*(| 4)	C	56	0.00022	1.38867
999.	RY*(| 5)	C	56	0.00013	1.83983
1000.	RY*(| 6)	C	56	0.00010	1.74745
1001.	RY*(| 7)	C	56	0.00004	1.61105
1002.	RY*(| 8)	C	56	0.00005	2.25446
1003.	RY*(| 9)	C	56	0.00003	2.25304
1004.	RY*(| 10)	C	56	0.00001	2.04739
1005.	RY*(| 11)	C	56	0.00001	2.44828
1006.	RY*(| 12)	C	56	0.00001	2.46074
1007.	RY*(| 13)	C	56	0.00001	2.05515
1008.	RY*(| 14)	C	56	0.00000	20.55252
1009.	RY*(| 1)	C	57	0.00187	0.77907
1010.	RY*(| 2)	C	57	0.00134	0.85389
1011.	RY*(| 3)	C	57	0.00047	1.11156
1012.	RY*(| 4)	C	57	0.00025	1.36688
1013.	RY*(| 5)	C	57	0.00018	1.58546
1014.	RY*(| 6)	C	57	0.00015	1.71453
1015.	RY*(| 7)	C	57	0.00008	2.19414
1016.	RY*(| 8)	C	57	0.00006	2.03248
1017.	RY*(| 9)	C	57	0.00002	2.37263
1018.	RY*(| 10)	C	57	0.00003	2.00210
1019.	RY*(| 11)	C	57	0.00002	2.54372
1020.	RY*(| 12)	C	57	0.00001	2.32326
1021.	RY*(| 13)	C	57	0.00000	20.15294
1022.	RY*(| 14)	C	57	0.00000	2.03972
1023.	RY*(| 1)	C	58	0.00156	0.94167
1024.	RY*(| 2)	C	58	0.00112	0.89956

1025.	RY*(| 3)	C	58	0.00046	0.83136
1026.	RY*(| 4)	C	58	0.00018	1.37691
1027.	RY*(| 5)	C	58	0.00014	1.56610
1028.	RY*(| 6)	C	58	0.00010	1.86396
1029.	RY*(| 7)	C	58	0.00006	2.20712
1030.	RY*(| 8)	C	58	0.00004	1.37507
1031.	RY*(| 9)	C	58	0.00004	2.29307
1032.	RY*(| 10)	C	58	0.00001	2.21946
1033.	RY*(| 11)	C	58	0.00001	2.39688
1034.	RY*(| 12)	C	58	0.00001	2.45795
1035.	RY*(| 13)	C	58	0.00001	2.08113
1036.	RY*(| 14)	C	58	0.00000	20.38982
1037.	RY*(| 1)	C	59	0.00167	0.85200
1038.	RY*(| 2)	C	59	0.00108	0.91695
1039.	RY*(| 3)	C	59	0.00050	0.87151
1040.	RY*(| 4)	C	59	0.00021	1.09802
1041.	RY*(| 5)	C	59	0.00016	1.67367
1042.	RY*(| 6)	C	59	0.00010	2.17597
1043.	RY*(| 7)	C	59	0.00008	2.26738
1044.	RY*(| 8)	C	59	0.00005	1.71348
1045.	RY*(| 9)	C	59	0.00004	1.73874
1046.	RY*(| 10)	C	59	0.00001	2.45796
1047.	RY*(| 11)	C	59	0.00001	2.51727
1048.	RY*(| 12)	C	59	0.00000	20.37556
1049.	RY*(| 13)	C	59	0.00001	2.22918
1050.	RY*(| 14)	C	59	0.00001	1.93934
1051.	RY*(| 1)	C	60	0.00173	0.89556
1052.	RY*(| 2)	C	60	0.00133	0.86446
1053.	RY*(| 3)	C	60	0.00047	1.12367
1054.	RY*(| 4)	C	60	0.00023	1.13161
1055.	RY*(| 5)	C	60	0.00019	1.80186
1056.	RY*(| 6)	C	60	0.00011	1.65999
1057.	RY*(| 7)	C	60	0.00006	2.30291
1058.	RY*(| 8)	C	60	0.00003	1.65011
1059.	RY*(| 9)	C	60	0.00004	2.63925
1060.	RY*(| 10)	C	60	0.00001	2.11372
1061.	RY*(| 11)	C	60	0.00001	2.52982
1062.	RY*(| 12)	C	60	0.00001	2.09279
1063.	RY*(| 13)	C	60	0.00001	2.32428
1064.	RY*(| 14)	C	60	0.00000	20.27242
1065.	RY*(| 1)	C	61	0.00159	0.95042
1066.	RY*(| 2)	C	61	0.00108	0.92611
1067.	RY*(| 3)	C	61	0.00046	0.80289
1068.	RY*(| 4)	C	61	0.00019	1.52112
1069.	RY*(| 5)	C	61	0.00014	1.58120
1070.	RY*(| 6)	C	61	0.00010	1.77457
1071.	RY*(| 7)	C	61	0.00006	2.16186
1072.	RY*(| 8)	C	61	0.00004	1.47399
1073.	RY*(| 9)	C	61	0.00004	2.35566
1074.	RY*(| 10)	C	61	0.00001	2.25826
1075.	RY*(| 11)	C	61	0.00001	2.24594
1076.	RY*(| 12)	C	61	0.00001	2.25334
1077.	RY*(| 13)	C	61	0.00000	20.52730
1078.	RY*(| 14)	C	61	0.00001	2.30590
1079.	RY*(| 1)	C	62	0.00178	0.81163
1080.	RY*(| 2)	C	62	0.00127	0.85863
1081.	RY*(| 3)	C	62	0.00040	1.07542
1082.	RY*(| 4)	C	62	0.00023	1.26309
1083.	RY*(| 5)	C	62	0.00016	1.61807
1084.	RY*(| 6)	C	62	0.00012	1.54980
1085.	RY*(| 7)	C	62	0.00007	2.17064
1086.	RY*(| 8)	C	62	0.00007	2.06883
1087.	RY*(| 9)	C	62	0.00003	2.49295
1088.	RY*(| 10)	C	62	0.00004	2.06901
1089.	RY*(| 11)	C	62	0.00000	20.24689
1090.	RY*(| 12)	C	62	0.00001	2.15050
1091.	RY*(| 13)	C	62	0.00001	2.24099
1092.	RY*(| 14)	C	62	0.00001	2.27253
1093.	RY*(| 1)	H	63	0.00043	1.79385
1094.	RY*(| 2)	H	63	0.00028	1.61778
1095.	RY*(| 3)	H	63	0.00011	1.97496

1096.	RY*(| 4)	H	63	0.00010	1.16266
1097.	RY*(| 5)	H	63	0.00003	2.44092
1098.	RY*(| 1)	H	64	0.00043	1.76821
1099.	RY*(| 2)	H	64	0.00028	1.64487
1100.	RY*(| 3)	H	64	0.00011	1.93275
1101.	RY*(| 4)	H	64	0.00010	1.10422
1102.	RY*(| 5)	H	64	0.00003	2.47834
1103.	RY*(| 1)	H	65	0.00120	0.61556
1104.	RY*(| 2)	H	65	0.00029	1.81621
1105.	RY*(| 3)	H	65	0.00026	2.07594
1106.	RY*(| 4)	H	65	0.00011	2.02815
1107.	RY*(| 5)	H	65	0.00004	2.72868
1108.	RY*(| 1)	H	66	0.00029	1.22356
1109.	RY*(| 2)	H	66	0.00022	1.61908
1110.	RY*(| 3)	H	66	0.00018	1.12419
1111.	RY*(| 4)	H	66	0.00012	2.03314
1112.	RY*(| 5)	H	66	0.00002	2.75975
1113.	RY*(| 1)	H	67	0.00103	0.62193
1114.	RY*(| 2)	H	67	0.00028	2.22492
1115.	RY*(| 3)	H	67	0.00024	1.68072
1116.	RY*(| 4)	H	67	0.00013	2.02673
1117.	RY*(| 5)	H	67	0.00004	2.73532
1118.	RY*(| 1)	H	68	0.00136	0.61408
1119.	RY*(| 2)	H	68	0.00033	2.05173
1120.	RY*(| 3)	H	68	0.00025	1.87159
1121.	RY*(| 4)	H	68	0.00011	2.02656
1122.	RY*(| 5)	H	68	0.00004	2.71909
1123.	RY*(| 1)	H	69	0.00031	1.11626
1124.	RY*(| 2)	H	69	0.00024	1.62513
1125.	RY*(| 3)	H	69	0.00018	1.21117
1126.	RY*(| 4)	H	69	0.00012	2.02311
1127.	RY*(| 5)	H	69	0.00002	2.74760
1128.	RY*(| 1)	H	70	0.00114	0.60560
1129.	RY*(| 2)	H	70	0.00027	2.22135
1130.	RY*(| 3)	H	70	0.00026	1.64416
1131.	RY*(| 4)	H	70	0.00011	2.01719
1132.	RY*(| 5)	H	70	0.00004	2.72522
1133.	RY*(| 1)	H	71	0.00044	1.79584
1134.	RY*(| 2)	H	71	0.00033	1.65195
1135.	RY*(| 3)	H	71	0.00012	1.99082
1136.	RY*(| 4)	H	71	0.00010	1.12205
1137.	RY*(| 5)	H	71	0.00003	2.49225
1138.	RY*(| 1)	H	72	0.00044	1.76929
1139.	RY*(| 2)	H	72	0.00033	1.64027
1140.	RY*(| 3)	H	72	0.00011	1.98835
1141.	RY*(| 4)	H	72	0.00010	1.10642
1142.	RY*(| 5)	H	72	0.00003	2.53827
1143.	RY*(| 1)	H	73	0.00131	0.61001
1144.	RY*(| 2)	H	73	0.00028	1.92813
1145.	RY*(| 3)	H	73	0.00026	1.94217
1146.	RY*(| 4)	H	73	0.00011	2.02867
1147.	RY*(| 5)	H	73	0.00004	2.73421
1148.	RY*(| 1)	H	74	0.00032	1.16703
1149.	RY*(| 2)	H	74	0.00023	1.62436
1150.	RY*(| 3)	H	74	0.00019	1.17402
1151.	RY*(| 4)	H	74	0.00012	2.02821
1152.	RY*(| 5)	H	74	0.00002	2.75731
1153.	RY*(| 1)	H	75	0.00114	0.61482
1154.	RY*(| 2)	H	75	0.00028	2.23038
1155.	RY*(| 3)	H	75	0.00024	1.66626
1156.	RY*(| 4)	H	75	0.00014	2.02840
1157.	RY*(| 5)	H	75	0.00004	2.73195
1158.	RY*(| 1)	H	76	0.00129	0.63414
1159.	RY*(| 2)	H	76	0.00032	2.13747
1160.	RY*(| 3)	H	76	0.00024	1.78842
1161.	RY*(| 4)	H	76	0.00013	2.04052
1162.	RY*(| 5)	H	76	0.00004	2.72664
1163.	RY*(| 1)	H	77	0.00031	1.12293
1164.	RY*(| 2)	H	77	0.00022	1.61640
1165.	RY*(| 3)	H	77	0.00019	1.22559
1166.	RY*(| 4)	H	77	0.00012	2.02405

1167.	RY*(| 5)	H	77	0.00002	2.75728
1168.	RY*(| 1)	H	78	0.00125	0.61110
1169.	RY*(| 2)	H	78	0.00026	2.22938
1170.	RY*(| 3)	H	78	0.00026	1.64339
1171.	RY*(| 4)	H	78	0.00011	2.02722
1172.	RY*(| 5)	H	78	0.00004	2.72698
1173.	RY*(| 1)	H	79	0.00168	0.86938
1174.	RY*(| 2)	H	79	0.00027	2.22307
1175.	RY*(| 3)	H	79	0.00017	1.90409
1176.	RY*(| 4)	H	79	0.00013	2.22953
1177.	RY*(| 5)	H	79	0.00001	2.89150
1178.	RY*(| 1)	H	80	0.00357	0.77119
1179.	RY*(| 2)	H	80	0.00027	2.43558
1180.	RY*(| 3)	H	80	0.00017	2.06186
1181.	RY*(| 4)	H	80	0.00013	1.99285
1182.	RY*(| 5)	H	80	0.00002	2.83084
1183.	RY*(| 1)	H	81	0.00179	0.83363
1184.	RY*(| 2)	H	81	0.00029	2.22266
1185.	RY*(| 3)	H	81	0.00019	1.94847
1186.	RY*(| 4)	H	81	0.00013	2.15321
1187.	RY*(| 5)	H	81	0.00002	2.84379
1188.	RY*(| 1)	H	82	0.00302	0.74587
1189.	RY*(| 2)	H	82	0.00024	2.40850
1190.	RY*(| 3)	H	82	0.00018	2.02148
1191.	RY*(| 4)	H	82	0.00013	2.03038
1192.	RY*(| 5)	H	82	0.00002	2.82438
1193.	RY*(| 1)	H	83	0.00174	0.80812
1194.	RY*(| 2)	H	83	0.00026	2.20093
1195.	RY*(| 3)	H	83	0.00018	1.90637
1196.	RY*(| 4)	H	83	0.00012	2.22428
1197.	RY*(| 5)	H	83	0.00002	2.86428
1198.	RY*(| 1)	H	84	0.00176	0.71425
1199.	RY*(| 2)	H	84	0.00023	2.35259
1200.	RY*(| 3)	H	84	0.00017	1.98275
1201.	RY*(| 4)	H	84	0.00013	2.06637
1202.	RY*(| 5)	H	84	0.00002	2.79829
1203.	RY*(| 1)	H	85	0.00183	0.77740
1204.	RY*(| 2)	H	85	0.00029	2.22606
1205.	RY*(| 3)	H	85	0.00018	1.93892
1206.	RY*(| 4)	H	85	0.00012	2.12847
1207.	RY*(| 5)	H	85	0.00002	2.81012
1208.	RY*(| 1)	H	86	0.00160	0.73705
1209.	RY*(| 2)	H	86	0.00025	2.16107
1210.	RY*(| 3)	H	86	0.00017	1.91241
1211.	RY*(| 4)	H	86	0.00012	2.13962
1212.	RY*(| 5)	H	86	0.00002	2.82939
1213.	RY*(| 1)	H	87	0.00064	0.70953
1214.	RY*(| 2)	H	87	0.00019	1.88972
1215.	RY*(| 3)	H	87	0.00012	1.78807
1216.	RY*(| 4)	H	87	0.00007	1.74216
1217.	RY*(| 5)	H	87	0.00002	2.71698
1218.	RY*(| 1)	H	88	0.00071	0.89578
1219.	RY*(| 2)	H	88	0.00024	1.79490
1220.	RY*(| 3)	H	88	0.00012	1.80289
1221.	RY*(| 4)	H	88	0.00007	1.71955
1222.	RY*(| 5)	H	88	0.00002	2.66637
1223.	RY*(| 1)	H	89	0.00090	1.12285
1224.	RY*(| 2)	H	89	0.00019	1.85056
1225.	RY*(| 3)	H	89	0.00012	1.86311
1226.	RY*(| 4)	H	89	0.00010	1.90580
1227.	RY*(| 5)	H	89	0.00002	2.66958
1228.	RY*(| 1)	H	90	0.00064	0.73010
1229.	RY*(| 2)	H	90	0.00016	1.82400
1230.	RY*(| 3)	H	90	0.00013	1.85029
1231.	RY*(| 4)	H	90	0.00006	1.68790
1232.	RY*(| 5)	H	90	0.00002	2.67493
1233.	RY*(| 1)	H	91	0.00062	1.02755
1234.	RY*(| 2)	H	91	0.00015	1.81332
1235.	RY*(| 3)	H	91	0.00015	1.79976
1236.	RY*(| 4)	H	91	0.00004	1.63403
1237.	RY*(| 5)	H	91	0.00002	2.69566

1238. RY*(1) H 92	0.00089	0.80131
1239. RY*(2) H 92	0.00014	1.82345
1240. RY*(3) H 92	0.00013	1.76209
1241. RY*(4) H 92	0.00006	1.69734
1242. RY*(5) H 92	0.00002	2.72109
1243. RY*(1) H 93	0.00063	0.69790
1244. RY*(2) H 93	0.00014	1.79790
1245. RY*(3) H 93	0.00014	1.81959
1246. RY*(4) H 93	0.00006	1.68060
1247. RY*(5) H 93	0.00002	2.70103
1248. RY*(1) H 94	0.00076	0.91344
1249. RY*(2) H 94	0.00018	1.78692
1250. RY*(3) H 94	0.00015	1.79901
1251. RY*(4) H 94	0.00006	1.60698
1252. RY*(5) H 94	0.00002	2.66551
1253. RY*(1) H 95	0.00054	0.76418
1254. RY*(2) H 95	0.00014	1.83136
1255. RY*(3) H 95	0.00013	1.89822
1256. RY*(4) H 95	0.00007	1.59324
1257. RY*(5) H 95	0.00001	2.70840
1258. RY*(1) H 96	0.00077	0.62470
1259. RY*(2) H 96	0.00018	1.83649
1260. RY*(3) H 96	0.00013	1.80780
1261. RY*(4) H 96	0.00010	1.86326
1262. RY*(5) H 96	0.00002	2.73045
1263. RY*(1) H 97	0.00090	0.89192
1264. RY*(2) H 97	0.00025	2.41614
1265. RY*(3) H 97	0.00012	1.88045
1266. RY*(4) H 97	0.00009	1.86340
1267. RY*(5) H 97	0.00002	2.73974
1268. RY*(1) H 98	0.00071	0.98641
1269. RY*(2) H 98	0.00020	1.70195
1270. RY*(3) H 98	0.00014	1.89711
1271. RY*(4) H 98	0.00009	1.63643
1272. RY*(5) H 98	0.00002	2.67976
1273. RY*(1) H 99	0.00062	0.70536
1274. RY*(2) H 99	0.00014	1.80266
1275. RY*(3) H 99	0.00014	1.82016
1276. RY*(4) H 99	0.00006	1.68172
1277. RY*(5) H 99	0.00002	2.69190
1278. RY*(1) H 100	0.00080	0.86635
1279. RY*(2) H 100	0.00016	1.79842
1280. RY*(3) H 100	0.00015	1.81577
1281. RY*(4) H 100	0.00006	1.62492
1282. RY*(5) H 100	0.00002	2.66602
1283. RY*(1) H 101	0.00056	0.75690
1284. RY*(2) H 101	0.00013	1.92768
1285. RY*(3) H 101	0.00014	1.79989
1286. RY*(4) H 101	0.00007	1.61722
1287. RY*(5) H 101	0.00001	2.70993
1288. RY*(1) H 102	0.00060	0.73052
1289. RY*(2) H 102	0.00018	1.79870
1290. RY*(3) H 102	0.00013	1.74538
1291. RY*(4) H 102	0.00010	1.89615
1292. RY*(5) H 102	0.00002	2.72772
1293. RY*(1) H 103	0.00071	0.97446
1294. RY*(2) H 103	0.00022	2.50420
1295. RY*(3) H 103	0.00012	1.85293
1296. RY*(4) H 103	0.00008	1.90415
1297. RY*(5) H 103	0.00003	2.74695
1298. RY*(1) H 104	0.00076	0.92555
1299. RY*(2) H 104	0.00022	1.76298
1300. RY*(3) H 104	0.00014	1.91786
1301. RY*(4) H 104	0.00011	1.70568
1302. RY*(5) H 104	0.00002	2.69090
1303. RY*(1) H 105	0.00059	0.70072
1304. RY*(2) H 105	0.00014	1.77845
1305. RY*(3) H 105	0.00014	1.81145
1306. RY*(4) H 105	0.00006	1.67339
1307. RY*(5) H 105	0.00003	2.69450
1308. RY*(1) H 106	0.00053	0.71215

1309. RY*(2) H 106	0.00014	1.82376
1310. RY*(3) H 106	0.00013	1.86905
1311. RY*(4) H 106	0.00007	1.62568
1312. RY*(5) H 106	0.00002	2.69300
1313. RY*(1) H 107	0.00074	0.92496
1314. RY*(2) H 107	0.00020	1.78659
1315. RY*(3) H 107	0.00014	1.79177
1316. RY*(4) H 107	0.00006	1.55249
1317. RY*(5) H 107	0.00002	2.67933
1318. RY*(1) H 108	0.00076	0.64259
1319. RY*(2) H 108	0.00018	1.84225
1320. RY*(3) H 108	0.00013	1.80704
1321. RY*(4) H 108	0.00011	1.86115
1322. RY*(5) H 108	0.00002	2.71187
1323. RY*(1) H 109	0.00088	0.84659
1324. RY*(2) H 109	0.00020	1.75570
1325. RY*(3) H 109	0.00014	1.94752
1326. RY*(4) H 109	0.00009	1.75711
1327. RY*(5) H 109	0.00002	2.68362
1328. RY*(1) H 110	0.00066	0.90989
1329. RY*(2) H 110	0.00024	2.43109
1330. RY*(3) H 110	0.00014	1.91267
1331. RY*(4) H 110	0.00007	1.89506
1332. RY*(5) H 110	0.00002	2.73635
1333. RY*(1) H 111	0.00075	0.66146
1334. RY*(2) H 111	0.00017	1.84752
1335. RY*(3) H 111	0.00014	1.79931
1336. RY*(4) H 111	0.00009	1.79512
1337. RY*(5) H 111	0.00002	2.70555
1338. RY*(1) H 112	0.00085	0.84559
1339. RY*(2) H 112	0.00021	1.82039
1340. RY*(3) H 112	0.00015	1.85275
1341. RY*(4) H 112	0.00008	1.69433
1342. RY*(5) H 112	0.00002	2.68168
1343. RY*(1) H 113	0.00047	1.25220
1344. RY*(2) H 113	0.00015	1.85904
1345. RY*(3) H 113	0.00011	2.08192
1346. RY*(4) H 113	0.00005	1.84175
1347. RY*(5) H 113	0.00002	2.75513
1348. RY*(1) H 114	0.00064	0.69363
1349. RY*(2) H 114	0.00014	1.80121
1350. RY*(3) H 114	0.00014	1.81947
1351. RY*(4) H 114	0.00006	1.68962
1352. RY*(5) H 114	0.00002	2.69883
1353. RY*(1) H 115	0.00055	0.77470
1354. RY*(2) H 115	0.00013	1.92434
1355. RY*(3) H 115	0.00014	1.80773
1356. RY*(4) H 115	0.00007	1.58426
1357. RY*(5) H 115	0.00002	2.70666
1358. RY*(1) H 116	0.00078	0.89106
1359. RY*(2) H 116	0.00018	1.79692
1360. RY*(3) H 116	0.00015	1.80172
1361. RY*(4) H 116	0.00006	1.60334
1362. RY*(5) H 116	0.00002	2.67269
1363. RY*(1) H 117	0.00063	0.74818
1364. RY*(2) H 117	0.00016	1.82064
1365. RY*(3) H 117	0.00013	1.86209
1366. RY*(4) H 117	0.00006	1.69002
1367. RY*(5) H 117	0.00002	2.69143
1368. RY*(1) H 118	0.00088	0.79119
1369. RY*(2) H 118	0.00014	1.83336
1370. RY*(3) H 118	0.00013	1.77163
1371. RY*(4) H 118	0.00006	1.71378
1372. RY*(5) H 118	0.00002	2.71969
1373. RY*(1) H 119	0.00062	0.97863
1374. RY*(2) H 119	0.00015	1.82347
1375. RY*(3) H 119	0.00015	1.82648
1376. RY*(4) H 119	0.00005	1.67412
1377. RY*(5) H 119	0.00002	2.71322
1378. RY*(1) H 120	0.00056	0.80439
1379. RY*(2) H 120	0.00017	1.83674

1380. RY*(3) H 120	0.00013	1.76527
1381. RY*(4) H 120	0.00008	1.78266
1382. RY*(5) H 120	0.00002	2.71997
1383. RY*(1) H 121	0.00083	0.87271
1384. RY*(2) H 121	0.00020	2.40013
1385. RY*(3) H 121	0.00013	1.89478
1386. RY*(4) H 121	0.00006	1.84799
1387. RY*(5) H 121	0.00002	2.75149
1388. RY*(1) H 122	0.00073	0.83245
1389. RY*(2) H 122	0.00025	1.75042
1390. RY*(3) H 122	0.00013	1.90770
1391. RY*(4) H 122	0.00009	1.70012
1392. RY*(5) H 122	0.00002	2.72641
1393. RY*(1) H 123	0.00070	0.74128
1394. RY*(2) H 123	0.00020	1.88868
1395. RY*(3) H 123	0.00012	1.81763
1396. RY*(4) H 123	0.00007	1.75120
1397. RY*(5) H 123	0.00003	2.72200
1398. RY*(1) H 124	0.00073	0.86185
1399. RY*(2) H 124	0.00024	1.78412
1400. RY*(3) H 124	0.00012	1.83974
1401. RY*(4) H 124	0.00008	1.74178
1402. RY*(5) H 124	0.00002	2.65696
1403. RY*(1) H 125	0.00056	0.84236
1404. RY*(2) H 125	0.00017	1.94721
1405. RY*(3) H 125	0.00014	1.97302
1406. RY*(4) H 125	0.00007	1.80244
1407. RY*(5) H 125	0.00002	2.73228
1408. RY*(1) H 126	0.00062	0.75508
1409. RY*(2) H 126	0.00016	1.82932
1410. RY*(3) H 126	0.00012	1.86322
1411. RY*(4) H 126	0.00006	1.68041
1412. RY*(5) H 126	0.00002	2.69509
1413. RY*(1) H 127	0.00062	1.08144
1414. RY*(2) H 127	0.00017	1.78061
1415. RY*(3) H 127	0.00015	1.81164
1416. RY*(4) H 127	0.00005	1.66893
1417. RY*(5) H 127	0.00002	2.71974
1418. RY*(1) H 128	0.00088	0.78126
1419. RY*(2) H 128	0.00015	1.83365
1420. RY*(3) H 128	0.00013	1.79183
1421. RY*(4) H 128	0.00006	1.69953
1422. RY*(5) H 128	0.00002	2.72371
1423. RY*(1) H 129	0.00064	0.69535
1424. RY*(2) H 129	0.00014	1.81770
1425. RY*(3) H 129	0.00015	1.82297
1426. RY*(4) H 129	0.00006	1.67837
1427. RY*(5) H 129	0.00002	2.70271
1428. RY*(1) H 130	0.00079	0.87993
1429. RY*(2) H 130	0.00017	1.78541
1430. RY*(3) H 130	0.00015	1.80595
1431. RY*(4) H 130	0.00006	1.62807
1432. RY*(5) H 130	0.00002	2.67961
1433. RY*(1) H 131	0.00059	0.79981
1434. RY*(2) H 131	0.00013	1.92011
1435. RY*(3) H 131	0.00014	1.80174
1436. RY*(4) H 131	0.00007	1.59487
1437. RY*(5) H 131	0.00002	2.71060
1438. RY*(1) H 132	0.00076	0.60165
1439. RY*(2) H 132	0.00018	1.84445
1440. RY*(3) H 132	0.00014	1.82504
1441. RY*(4) H 132	0.00009	1.83983
1442. RY*(5) H 132	0.00002	2.72752
1443. RY*(1) H 133	0.00092	0.87791
1444. RY*(2) H 133	0.00023	2.37742
1445. RY*(3) H 133	0.00013	1.85754
1446. RY*(4) H 133	0.00008	1.82668
1447. RY*(5) H 133	0.00002	2.71545
1448. RY*(1) H 134	0.00075	0.92314
1449. RY*(2) H 134	0.00021	1.71696
1450. RY*(3) H 134	0.00014	1.87739

1451.	RY*(	4)	H	134			0.00009	1.66305
1452.	RY*(	5)	H	134			0.00002	2.68313
1453.	BD*(	1)	C	1	- O	2	0.04220	0.51533
1454.	BD*(	2)	C	1	- O	2	0.48062	0.04161 224(v),223(v),241(g),227(g) 231(g),247(g)
1455.	BD*(	1)	C	1	- B	14	0.11075	0.33338 1604(r),1484(g),1594(r) 1513(r),1601(r),1473(v) 1475(v),411(g),1597(r) 1589(r),1453(g)
1456.	BD*(	1)	C	1	- B	15	0.06815	0.45203
1457.	BD*(	1)	C	3	- C	4	0.03587	0.45910
1458.	BD*(	1)	C	3	- C	8	0.02327	0.47800
1459.	BD*(	2)	C	3	- C	8	0.33135	0.01402 1462(v),1467(v),1581(v) 326(g),1582(v)
1460.	BD*(	1)	C	3	- C	53	0.03220	0.33721
1461.	BD*(	1)	C	4	- C	5	0.03690	0.45890
1462.	BD*(	2)	C	4	- C	5	0.37359	0.00915 1467(v),1459(v),223(r) 1472(v),1474(v),1576(v) 1575(v),298(v),269(g)
1463.	BD*(	1)	C	4	- N	9	0.03921	0.30940
1464.	BD*(	1)	C	5	- C	6	0.02290	0.47118
1465.	BD*(	1)	C	5	- C	51	0.03210	0.32453
1466.	BD*(	1)	C	6	- C	7	0.01486	0.48888
1467.	BD*(	2)	C	6	- C	7	0.33555	0.00445 1462(v),1459(v),312(g) 298(g)
1468.	BD*(	1)	C	6	- H	78	0.01759	0.34499
1469.	BD*(	1)	C	7	- C	8	0.01498	0.48832
1470.	BD*(	1)	C	7	- H	77	0.01576	0.34484
1471.	BD*(	1)	C	8	- H	76	0.01781	0.35502
1472.	BD*(	1)	N	9	- C	10	0.04581	0.34876
1473.	BD*(	2)	N	9	- C	10	0.72110	-0.04497 1481(v),1455(v),353(g) 1461(v),1484(v),1457(v) 355(g)
1474.	BD*(	1)	N	9	- C	13	0.03014	0.34314
1475.	BD*(	1)	C	10	- N	11	0.04659	0.34712
1476.	BD*(	1)	C	10	- B	14	0.02957	0.44002
1477.	BD*(	1)	N	11	- C	12	0.02954	0.34108
1478.	BD*(	1)	N	11	- C	41	0.03975	0.30683
1479.	BD*(	2)	N	11	- C	41	0.45441	0.99640 858(v),802(v),1550(g) 1549(g),794(g),788(g),800(v) 789(g),787(g),792(g),856(v) 884(r),996(r),1551(g),842(r) 870(r),793(g),809(v),869(r) 790(g),844(r),816(r),855(v) 805(v),865(v),366(g),867(v) 828(r),338(r),1560(v),897(r) 1024(r),857(v),913(r),811(v) 866(v),1552(v),372(g) 1413(r),861(v),871(r),898(r) 912(r),907(r),832(r),813(r) 903(r),257(r),411(r),848(r) 835(r),819(r),1030(r),853(r) 824(r),860(v),226(r),902(r) 409(r),799(v),850(r),801(v) 864(v),1293(r),808(v),890(r)
1480.	BD*(	1)	C	12	- C	13	0.00980	0.50420
1481.	BD*(	2)	C	12	- C	13	0.28111	-0.01244 1473(v),384(g),398(g)
1482.	BD*(	1)	C	12	- H	71	0.01213	0.33596
1483.	BD*(	1)	C	13	- H	72	0.01229	0.33598
1484.	BD*(	1)	B	14	- B	15	0.04014	0.48411
1485.	BD*(	1)	B	15	- C	16	0.05483	0.40975
1486.	BD*(	1)	C	16	- N	17	0.04814	0.35327
1487.	BD*(	2)	C	16	- N	17	0.60501	-0.05833 224(v),1492(v),437(g) 1498(v),438(g),1497(v) 223(r)
1488.	BD*(	1)	C	16	- N	20	0.05247	0.35270
1489.	BD*(	1)	N	17	- C	18	0.03043	0.33474
1490.	BD*(	1)	N	17	- C	21	0.04192	0.28877
1491.	BD*(	1)	C	18	- C	19	0.00978	0.47647
1492.	BD*(	2)	C	18	- C	19	0.28227	-0.03212 1487(v),468(g),482(g)
1493.	BD*(	1)	C	18	- H	63	0.01214	0.31976

1494.	BD*(	1)	C	19 -	N	20	0.03069	0.32900
1495.	BD*(	1)	C	19 -	H	64	0.01258	0.31713
1496.	BD*(	1)	N	20 -	C	31	0.04104	0.28946
1497.	BD*(	1)	C	21 -	C	22	0.03442	0.45657
1498.	BD*(	1)	C	21 -	C	26	0.03531	0.45647
1499.	BD*(	2)	C	21 -	C	26	0.38598	0.00727 1506(v),1501(v),1486(v) 1489(v),1518(v),1517(v) 564(v),507(g)
1500.	BD*(	1)	C	22 -	C	23	0.02275	0.47953
1501.	BD*(	2)	C	22 -	C	23	0.32447	0.01569 1499(v),1506(v),1511(v) 536(g),1512(v)
1502.	BD*(	1)	C	22 -	C	27	0.03210	0.33217
1503.	BD*(	1)	C	23 -	C	24	0.01470	0.49071
1504.	BD*(	1)	C	23 -	H	67	0.01740	0.35479
1505.	BD*(	1)	C	24 -	C	25	0.01474	0.48984
1506.	BD*(	2)	C	24 -	C	25	0.33515	0.00573 1499(v),1501(v),550(g) 564(g)
1507.	BD*(	1)	C	24 -	H	66	0.01546	0.34666
1508.	BD*(	1)	C	25 -	C	26	0.02276	0.47081
1509.	BD*(	1)	C	25 -	H	65	0.01723	0.34672
1510.	BD*(	1)	C	26 -	C	29	0.03221	0.32251
1511.	BD*(	1)	C	27 -	C	28	0.01812	0.28612
1512.	BD*(	1)	C	27 -	C	62	0.01403	0.30271
1513.	BD*(	1)	C	27 -	H	84	0.02449	0.32569
1514.	BD*(	1)	C	28 -	H	90	0.00804	0.32412
1515.	BD*(	1)	C	28 -	H	91	0.00798	0.32860
1516.	BD*(	1)	C	28 -	H	92	0.01047	0.32142
1517.	BD*(	1)	C	29 -	C	30	0.01761	0.28142
1518.	BD*(	1)	C	29 -	C	61	0.01761	0.28775
1519.	BD*(	1)	C	29 -	H	83	0.02465	0.31304
1520.	BD*(	1)	C	30 -	H	93	0.00762	0.31884
1521.	BD*(	1)	C	30 -	H	94	0.01056	0.31590
1522.	BD*(	1)	C	30 -	H	95	0.00687	0.32035
1523.	BD*(	1)	C	31 -	C	32	0.03513	0.44686
1524.	BD*(	1)	C	31 -	C	36	0.03523	0.45149
1525.	BD*(	2)	C	31 -	C	36	0.37263	0.00103 1527(v),1532(v),1543(v) 1494(v),1488(v),1544(v) 647(g),704(v)
1526.	BD*(	1)	C	32 -	C	33	0.02267	0.46340
1527.	BD*(	2)	C	32 -	C	33	0.34032	0.00070 1525(v),1532(v),1538(v) 1537(v),676(g)
1528.	BD*(	1)	C	32 -	C	37	0.03229	0.31681
1529.	BD*(	1)	C	33 -	C	34	0.01475	0.47915
1530.	BD*(	1)	C	33 -	H	70	0.01721	0.33927
1531.	BD*(	1)	C	34 -	C	35	0.01478	0.47953
1532.	BD*(	2)	C	34 -	C	35	0.33303	-0.00352 1527(v),1525(v),690(g) 704(g)
1533.	BD*(	1)	C	34 -	H	69	0.01550	0.33870
1534.	BD*(	1)	C	35 -	C	36	0.02305	0.46508
1535.	BD*(	1)	C	35 -	H	68	0.01717	0.34235
1536.	BD*(	1)	C	36 -	C	39	0.03217	0.32192
1537.	BD*(	1)	C	37 -	C	38	0.01669	0.27981
1538.	BD*(	1)	C	37 -	C	55	0.01793	0.28432
1539.	BD*(	1)	C	37 -	H	85	0.02520	0.30853
1540.	BD*(	1)	C	38 -	H	105	0.00720	0.31659
1541.	BD*(	1)	C	38 -	H	106	0.00679	0.31780
1542.	BD*(	1)	C	38 -	H	107	0.01082	0.31202
1543.	BD*(	1)	C	39 -	C	40	0.01773	0.28181
1544.	BD*(	1)	C	39 -	C	56	0.01637	0.29369
1545.	BD*(	1)	C	39 -	H	86	0.02379	0.31526
1546.	BD*(	1)	C	40 -	H	99	0.00750	0.32021
1547.	BD*(	1)	C	40 -	H	100	0.01046	0.31551
1548.	BD*(	1)	C	40 -	H	101	0.00695	0.32045
1549.	BD*(	1)	C	41 -	C	42	0.02999	0.63774
1550.	BD*(	1)	C	41 -	C	46	0.03084	0.63927
1551.	BD*(	2)	C	41 -	C	46	0.37132	0.02626 1553(v),1558(v),223(r) 1479(g),1475(v),1569(v) 1477(v),1549(g),1570(v) 1550(g),787(g),843(v),788(g)
1552.	BD*(	1)	C	42 -	C	43	0.02303	0.47717
1553.	BD*(	2)	C	42 -	C	43	0.33091	0.01298 1558(v),1551(v),1563(v)

								814(g),1564(v),815(g)
1554.	BD*(	1)	C	42	- C	47	0.03204	0.33798
1555.	BD*(	1)	C	43	- C	44	0.01506	0.48865
1556.	BD*(	1)	C	43	- H	75	0.01779	0.35502
1557.	BD*(	1)	C	44	- C	45	0.01496	0.48977
1558.	BD*(	2)	C	44	- C	45	0.33468	0.00403 1553(v),1551(v),829(g) 843(g)
1559.	BD*(	1)	C	44	- H	74	0.01582	0.34526
1560.	BD*(	1)	C	45	- C	46	0.02319	0.47103
1561.	BD*(	1)	C	45	- H	73	0.01777	0.34587
1562.	BD*(	1)	C	46	- C	49	0.03202	0.32583
1563.	BD*(	1)	C	47	- C	48	0.01776	0.29402
1564.	BD*(	1)	C	47	- C	57	0.01407	0.30738
1565.	BD*(	1)	C	47	- H	80	0.02568	0.35553
1566.	BD*(	1)	C	48	- H	126	0.00771	0.33477
1567.	BD*(	1)	C	48	- H	127	0.00801	0.33974
1568.	BD*(	1)	C	48	- H	128	0.01041	0.32767
1569.	BD*(	1)	C	49	- C	50	0.01781	0.28319
1570.	BD*(	1)	C	49	- C	58	0.01742	0.28894
1571.	BD*(	1)	C	49	- H	79	0.02452	0.32096
1572.	BD*(	1)	C	50	- H	129	0.00762	0.32054
1573.	BD*(	1)	C	50	- H	130	0.01064	0.31734
1574.	BD*(	1)	C	50	- H	131	0.00691	0.32406
1575.	BD*(	1)	C	51	- C	52	0.01736	0.28291
1576.	BD*(	1)	C	51	- C	59	0.01808	0.28864
1577.	BD*(	1)	C	51	- H	81	0.02484	0.31987
1578.	BD*(	1)	C	52	- H	114	0.00758	0.32098
1579.	BD*(	1)	C	52	- H	115	0.00682	0.32379
1580.	BD*(	1)	C	52	- H	116	0.01069	0.31728
1581.	BD*(	1)	C	53	- C	54	0.01793	0.29367
1582.	BD*(	1)	C	53	- C	60	0.01440	0.30966
1583.	BD*(	1)	C	53	- H	82	0.02457	0.35020
1584.	BD*(	1)	C	54	- H	117	0.00781	0.33391
1585.	BD*(	1)	C	54	- H	118	0.01050	0.32745
1586.	BD*(	1)	C	54	- H	119	0.00765	0.33710
1587.	BD*(	1)	C	55	- H	108	0.00767	0.32215
1588.	BD*(	1)	C	55	- H	109	0.01032	0.31999
1589.	BD*(	1)	C	55	- H	110	0.00695	0.34672
1590.	BD*(	1)	C	56	- H	102	0.00705	0.32957
1591.	BD*(	1)	C	56	- H	103	0.00748	0.35656
1592.	BD*(	1)	C	56	- H	104	0.01059	0.32491
1593.	BD*(	1)	C	57	- H	123	0.00670	0.35046
1594.	BD*(	1)	C	57	- H	124	0.01162	0.33261
1595.	BD*(	1)	C	57	- H	125	0.00660	0.34904
1596.	BD*(	1)	C	58	- H	132	0.00758	0.32308
1597.	BD*(	1)	C	58	- H	133	0.00692	0.34711
1598.	BD*(	1)	C	58	- H	134	0.01074	0.31874
1599.	BD*(	1)	C	59	- H	111	0.00771	0.32248
1600.	BD*(	1)	C	59	- H	112	0.01068	0.31907
1601.	BD*(	1)	C	59	- H	113	0.00685	0.34276
1602.	BD*(	1)	C	60	- H	120	0.00651	0.35076
1603.	BD*(	1)	C	60	- H	121	0.00663	0.36399
1604.	BD*(	1)	C	60	- H	122	0.01163	0.33398
1605.	BD*(	1)	C	61	- H	96	0.00764	0.32425
1606.	BD*(	1)	C	61	- H	97	0.00685	0.34830
1607.	BD*(	1)	C	61	- H	98	0.01033	0.32136
1608.	BD*(	1)	C	62	- H	87	0.00677	0.33607
1609.	BD*(	1)	C	62	- H	88	0.01126	0.32918
1610.	BD*(	1)	C	62	- H	89	0.00967	0.36987

Total Lewis	436.90072	(97.5225%)
Valence non-Lewis	10.37751	(2.3164%)
Rydberg non-Lewis	0.72177	(0.1611%)
Total unit 1	448.00000	(100.0000%)
Charge unit 1	0.00000	

NATURAL LOCALIZED MOLECULAR ORBITAL (NLMO) ANALYSIS:

Highest occupied NBOs are not at the beginning of the NBO list;

```
The NLMO program is not currently set up to handle this.
Sorting of NBOs:                  160  178  175  169  167  174  168  177  176  189
Sorting of NBOs:                  179  199  170  171  162  195  187  197  209  207
Sorting of NBOs:                  190  194  159  185  184  192  204  163  196  180
Sorting of NBOs:                  191  200  193  188  198  161  208  210  211  205
Sorting of NBOs:                  202  165  186  182  213  217  203  164  216  183
Sorting of NBOs:                  219  201  166  181  212  206  214  215  220  218
Sorting of NBOs:                  172  173    1   36   34   37   42   44   23   22
Sorting of NBOs:                   20   25   38   11   26   39   28   79   77   72
Sorting of NBOs:                   71   74   82  105   14   53   46  103   17   51
Sorting of NBOs:                   45    9   56  108   12   48    5  100    6  221
Sorting of NBOs:                   76   84   58  110   13   50   85  102    8   65
Sorting of NBOs:                   86   91  117  123  124   66  118   92   59   60
Sorting of NBOs:                  112  130  129  111   43   41   24   33   31   30
Sorting of NBOs:                   81   78   83  109   16  107   57   18   55  104
Sorting of NBOs:                   19   52   90   89   88   69   95   70   96   68
Sorting of NBOs:                  128  121   94  122  127  126  120   63  136  148
Sorting of NBOs:                  146  155  135  147   64  144   62  153  149  145
Sorting of NBOs:                  137  140  154  134  115   87  133  138  116  132
Sorting of NBOs:                   67  142  157  114  139  125  152   93  119  156
Sorting of NBOs:                  143  141  151  158  150   61   97    4  131  113
Sorting of NBOs:                   98    3   35   32   21   40    2  225   29   73
Sorting of NBOs:                   80   27   75   47   10  106   15   54  101    7
Sorting of NBOs:                   49   99  222 1487 1473 1492 1481 1532 1527 1525
Sorting of NBOs:                 1558 1467 1506 1499 1462 1553 1459 1501 1551  224
Sorting of NBOs:                  223 1454 1537 1517 1543 1575 1569 1538 1511 1518
Sorting of NBOs:                 1576 1490 1570 1496 1581 1544 1563 1512 1478 1564
Sorting of NBOs:                 1539 1463 1582 1542 1519 1545 1547 1521 1540 1528
Sorting of NBOs:                 1495 1580 1573 1541 1598 1520 1600 1493 1577 1588
Sorting of NBOs:                 1546 1522 1548 1572 1571 1578 1607 1516 1536 1587
Sorting of NBOs:                 1599 1510 1596 1579 1574 1514 1605 1465 1592 1513
Sorting of NBOs:                 1562 1585 1568 1515 1494 1609 1590 1502 1594 1455
Sorting of NBOs:                 1584 1604 1489 1566 1482 1483 1608 1586 1460 1554
Sorting of NBOs:                 1533 1530 1567 1477 1535 1601 1474 1470 1468 1559
Sorting of NBOs:                 1561 1507 1589 1509 1597 1475 1606 1472 1595 1583
Sorting of NBOs:                 1593 1602 1488 1486 1504 1556 1471 1565 1591 1603
Sorting of NBOs:                 1610 1485 1476 1523 1524 1456 1498 1497 1461 1457
Sorting of NBOs:                 1526 1534 1508 1560 1464 1491 1552 1458 1529 1500
Sorting of NBOs:                 1531 1484 1469 1555 1466 1557 1505 1503 1480 1453
Sorting of NBOs:                  843  298  312  829  564  550  704  231  690  478
Sorting of NBOs:                 1438 1128 1143 1168 1118 1153 1103  464 1113 1258
Sorting of NBOs:                 1158 1549 1550 1318 1333  394  380  410  521 1348
Sorting of NBOs:                 1423 1243 1303 1273 1213 1308 1198  243  326 1228
Sorting of NBOs:                 1288  676 1208  857 1393  647  451  814 1188 1363
Sorting of NBOs:                  269 1408  507 1283 1253  744 1178 1353 1203 1009
Sorting of NBOs:                 1418  632  939  787  718  241  911 1368  256  577
Sorting of NBOs:                  940  745 1433  772 1238 1067 1378  366 1193 1079
Sorting of NBOs:                  912  424  633  801 1025 1388 1183  493 1403  536
Sorting of NBOs:                 1338 1323  997 1037  535 1010  240 1080  338 1398
Sorting of NBOs:                 1052 1278  773 1173 1039 1383  662 1443  604 1428
Sorting of NBOs:                  967  425  605  884 1358 1263 1051 1218  230  883
Sorting of NBOs:                  284  815 1024  968 1328 1248  983 1038 1448 1313
Sorting of NBOs:                 1298  675 1066  661  996 1023  995  981 1065  452
Sorting of NBOs:                  283  522  982 1293  899 1373  927  508 1268  325
Sorting of NBOs:                  858 1479  663  719  802  226  591  285 1233  634
Sorting of NBOs:                  620  941  494  913  257  732  746  953  869  453
Sorting of NBOs:                  800  523  557  578  396  340  382  871  777  590
Sorting of NBOs:                  356 1081  749  495  368 1413  703  255  480  648
Sorting of NBOs:                  774  369 1040  563  579  885  835  760 1101 1141
Sorting of NBOs:                  297  842  954  758 1011  730  466  897  618  717
Sorting of NBOs:                 1123  925  637 1136 1223 1163  870 1053  409 1110
Sorting of NBOs:                  969 1054  606  856  397  481  270  830 1096  467
Sorting of NBOs:                 1148 1150  305  955  902  828  827  689  623  688
Sorting of NBOs:                  310  383  311  549  696 1125  411  984  548  691
Sorting of NBOs:                 1108 1165  930  426  437  944 1343  242  506 1082
Sorting of NBOs:                  551  956  479  786  683  520  677  646  816  327
Sorting of NBOs:                  844  395  415  299  569  537  465  705  381  972
Sorting of NBOs:                  698  735  916  872  268  254  423 1012  799  431
Sorting of NBOs:                  565 1030 1026  341  320  763  716  492  998  339
Sorting of NBOs:                  702  855  660  576  282  324  888  357  841  674
Sorting of NBOs:                  813  609  296  562  534  484  367  314  754  833
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Sorting of NBOs: 485 438 271 593 594 971 788 421 353 318
Sorting of NBOs: 1072 607 450 543 850 611 837 319 483 810
Sorting of NBOs: 333 946 898 592 470 727 655 385 926 386
Sorting of NBOs: 408 439 469 265 1068 399 440 708 886 988
Sorting of NBOs: 435 739 442 401 821 1084 1316 731 471 759
Sorting of NBOs: 1027 619 695 555 359 293 775 866 387 1069
Sorting of NBOs: 665 1356 1013 641 355 792 915 1256 1436 974
Sorting of NBOs: 400 936 649 259 742 1361 680 823 427 789
Sorting of NBOs: 1251 793 570 1001 762 874 1164 734 1286 1094
Sorting of NBOs: 958 1083 1109 848 1149 1281 1124 1311 595 443
Sorting of NBOs: 1431 671 422 541 1236 1271 747 942 558 1139
Sorting of NBOs: 531 313 1170 1130 441 352 304 1099 914 653
Sorting of NBOs: 544 1058 635 1134 509 1056 804 1451 1155 1416
Sorting of NBOs: 513 1306 1041 1376 354 1426 1411 1246 1115 1276
Sorting of NBOs: 1231 622 574 1351 1366 737 525 236 1341 276
Sorting of NBOs: 710 1241 629 1421 1391 1269 1301 336 901 275
Sorting of NBOs: 713 1044 1371 1014 587 1449 1221 720 770 852
Sorting of NBOs: 820 554 847 582 790 417 331 468 515 851
Sorting of NBOs: 909 1045 482 1401 1216 288 1290 985 1000 624
Sorting of NBOs: 258 1389 694 1396 552 929 1324 1326 714 765
Sorting of NBOs: 302 234 943 819 1240 1299 229 1380 681 722
Sorting of NBOs: 384 1098 1138 860 398 685 1370 330 447 934
Sorting of NBOs: 524 1070 920 861 766 1304 932 1414 287 890
Sorting of NBOs: 1381 1399 1429 1314 1249 1215 1160 476 512 1315
Sorting of NBOs: 1420 1093 1219 1336 1133 803 1359 1244 1279 1289
Sorting of NBOs: 1250 794 1335 1235 1285 1349 1360 1435 986 1055
Sorting of NBOs: 1406 1274 1220 1430 1320 1355 1260 1305 1415 709
Sorting of NBOs: 1234 1280 692 1104 1395 873 1424 322 711 316
Sorting of NBOs: 1350 1245 1275 900 1339 1364 436 651 306 957
Sorting of NBOs: 636 1425 1239 1374 761 1309 1229 1440 412 581
Sorting of NBOs: 1375 1446 889 580 560 1409 277 1254 335 849
Sorting of NBOs: 1369 1419 1259 1379 780 666 723 601 402 1400
Sorting of NBOs: 1441 999 307 701 667 1346 568 805 1319 859
Sorting of NBOs: 1439 598 678 1334 1386 1230 1224 488 1340 863
Sorting of NBOs: 1295 904 627 959 428 621 791 1445 733 862
Sorting of NBOs: 664 1344 1321 807 1365 566 1225 538 1410 1261
Sorting of NBOs: 1266 1028 834 721 1310 289 1120 895 991 300
Sorting of NBOs: 389 1450 928 1265 290 845 583 650 950 1394
Sorting of NBOs: 328 1214 977 286 706 540 817 831 1385 1331
Sorting of NBOs: 1291 1270 527 545 1255 363 764 668 1175 1296
Sorting of NBOs: 1226 1195 776 652 1390 781 1210 358 1330 272
Sorting of NBOs: 429 879 490 1300 514 1434 887 1354 1284 1144
Sorting of NBOs: 274 614 1100 528 473 526 876 260 1205 907
Sorting of NBOs: 1050 262 1145 906 806 596 1404 1325 1185 233
Sorting of NBOs: 767 390 573 839 654 610 964 973 922 487
Sorting of NBOs: 406 475 404 724 584 510 1405 597 1095 1200
Sorting of NBOs: 1140 608 625 1135 1181 615 896 840 963 600
Sorting of NBOs: 1018 935 796 877 273 261 279 918 628 903
Sorting of NBOs: 1131 945 303 1190 1126 1166 1121 1116 684 1171
Sorting of NBOs: 1106 1151 1156 1146 931 682 571 1191 750 1016
Sorting of NBOs: 517 511 1111 586 736 1022 1161 626 1004 923
Sorting of NBOs: 1119 784 1007 824 643 970 1180 227 1201 561
Sorting of NBOs: 1086 1088 785 1105 905 572 317 1035 1345 542
Sorting of NBOs: 961 1062 979 738 539 656 880 748 700 1060
Sorting of NBOs: 960 875 756 1206 818 321 640 768 933 1159
Sorting of NBOs: 975 978 1211 924 753 332 878 1090 1186 391
Sorting of NBOs: 329 891 1209 779 1071 962 825 1085 757 292
Sorting of NBOs: 1042 752 639 952 822 864 893 638 1015 599
Sorting of NBOs: 1194 612 1029 919 740 751 434 1032 1129 1184
Sorting of NBOs: 1174 1196 1114 392 1204 1049 1169 1176 1154 669
Sorting of NBOs: 725 617 496 948 342 1091 235 1075 228 1003
Sorting of NBOs: 1076 1002 686 989 642 361 1074 976 454 1043
Sorting of NBOs: 644 613 1092 949 990 782 370 308 445 1031
Sorting of NBOs: 1057 1078 489 474 809 1020 697 1063 670 263
Sorting of NBOs: 741 334 1199 264 602 529 1073 679 994 546
Sorting of NBOs: 769 405 707 630 894 532 1017 585 658 1444
Sorting of NBOs: 987 280 726 446 518 501 344 498 266 712
Sorting of NBOs: 1033 553 778 808 459 1384 811 588 908 881
Sorting of NBOs: 418 1189 232 836 937 372 965 832 728 1264
Sorting of NBOs: 315 291 456 657 294 797 371 1329 846 1179
Sorting of NBOs: 672 362 993 1097 867 530 1005 865 567 556

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Sorting of NBOs:                 1034 1046 1006  301  343  497  237  516 1102  278
Sorting of NBOs:                  693  448 1137 1087 1294  345 1047  853  795 1061
Sorting of NBOs:                  414 1142  374  455 1019  364  503  500  457  462
Sorting of NBOs:                  917  377  238 1059 1402  444 1252 1282 1222  486
Sorting of NBOs:                  502 1227 1362  350 1232 1317 1432 1272 1342 1452
Sorting of NBOs:                  403 1327 1302 1367 1277 1312  249 1307 1412 1237
Sorting of NBOs:                 1352 1247 1427 1337 1357 1257 1287 1437 1322 1377
Sorting of NBOs:                 1447 1217  375 1122 1372 1417 1382 1242 1397 1422
Sorting of NBOs:                 1132 1392 1162 1172 1442 1292 1107 1262  252 1157
Sorting of NBOs:                 1407 1147 1117 1332 1267  460 1297 1127 1387 1347
Sorting of NBOs:                 1167 1152 1112  378  349  388  461  472  376 1202
Sorting of NBOs:                  420  504 1207 1192 1212 1182  348 1187 1197 1177
Sorting of NBOs:                  947  250  245  346  360  247  432  347  251  373
Sorting of NBOs:                  246  413  458  499  433  248  419  244  416  430
Sorting of NBOs:                  951  783  921  645  239  755  449  365 1021  616
Sorting of NBOs:                 1089  980  892 1064 1048 1036  992 1077 1008  882
Sorting of NBOs:                  966  826  547  687  603  854  309  337  575  938
Sorting of NBOs:                  715  559  673  743  910  533  631  295  519  838
Sorting of NBOs:                  729  771  323  868  393  477  699  407  589  812
Sorting of NBOs:                  267  491  798  281  659  351  505  463  379  253
Reordering of NBOs for storage:   160  178  175  169  167  174  168  177  176  189
Reordering of NBOs for storage:   179  199  170  171  162  195  187  197  209  207
Reordering of NBOs for storage:   190  194  159  185  184  192  204  163  196  180
Reordering of NBOs for storage:   191  200  193  188  198  161  208  210  211  205
Reordering of NBOs for storage:   202  165  186  182  213  217  203  164  216  183
Reordering of NBOs for storage:   219  201  166  181  212  206  214  215  220  218
Reordering of NBOs for storage:   172  173    1   36   34   37   42   44   23   22
Reordering of NBOs for storage:    20   25   38   11   26   39   28   79   77   72
Reordering of NBOs for storage:    71   74   82  105   14   53   46  103   17   51
Reordering of NBOs for storage:    45    9   56  108   12   48    5  100    6  221
Reordering of NBOs for storage:    76   84   58  110   13   50   85  102    8   65
Reordering of NBOs for storage:    86   91  117  123  124   66  118   92   59   60
Reordering of NBOs for storage:   112  130  129  111   43   41   24   33   31   30
Reordering of NBOs for storage:    81   78   83  109   16  107   57   18   55  104
Reordering of NBOs for storage:    19   52   90   89   88   69   95   70   96   68
Reordering of NBOs for storage:   128  121   94  122  127  126  120   63  136  148
Reordering of NBOs for storage:   146  155  135  147   64  144   62  153  149  145
Reordering of NBOs for storage:   137  140  154  134  115   87  133  138  116  132
Reordering of NBOs for storage:    67  142  157  114  139  125  152   93  119  156
Reordering of NBOs for storage:   143  141  151  158  150   61   97    4  131  113
Reordering of NBOs for storage:    98    3   35   32   21   40    2  225   29   73
Reordering of NBOs for storage:    80   27   75   47   10  106   15   54  101    7
Reordering of NBOs for storage:    49   99  222  224 1487 1473 1492 1481 1532 1527
Reordering of NBOs for storage:  1525 1558 1467 1506 1499 1462 1553 1459 1501 1551
Reordering of NBOs for storage:   223 1454 1537 1517 1543 1575 1569 1538 1511 1518
Reordering of NBOs for storage:  1576 1490 1570 1496 1581 1544 1563 1512 1478 1564
Reordering of NBOs for storage:  1539 1463 1582 1542 1519 1545 1547 1521 1540 1528
Reordering of NBOs for storage:  1495 1580 1573 1541 1598 1520 1600 1493 1577 1588
Reordering of NBOs for storage:  1546 1522 1548 1572 1571 1578 1607 1516 1536 1587
Reordering of NBOs for storage:  1599 1510 1596 1579 1574 1514 1605 1465 1592 1513
Reordering of NBOs for storage:  1562 1585 1568 1515 1494 1609 1590 1502 1594 1455
Reordering of NBOs for storage:  1584 1604 1489 1566 1482 1483 1608 1586 1460 1554
Reordering of NBOs for storage:  1533 1530 1567 1477 1535 1601 1474 1470 1468 1559
Reordering of NBOs for storage:  1561 1507 1589 1509 1597 1475 1606 1472 1595 1583
Reordering of NBOs for storage:  1593 1602 1488 1486 1504 1556 1471 1565 1591 1603
Reordering of NBOs for storage:  1610 1485 1476 1523 1524 1456 1498 1497 1461 1457
Reordering of NBOs for storage:  1526 1534 1508 1560 1464 1491 1552 1458 1529 1500
Reordering of NBOs for storage:  1531 1484 1469 1555 1466 1557 1505 1503 1480 1453
Reordering of NBOs for storage:  1549 1550 1479  843  298  312  829  564  550  704
Reordering of NBOs for storage:   231  690  478 1438 1128 1143 1168 1118 1153 1103
Reordering of NBOs for storage:   464 1113 1258 1158 1318 1333  394  380  410  521
Reordering of NBOs for storage:  1348 1423 1243 1303 1273 1213 1308 1198  243  326
Reordering of NBOs for storage:  1228 1288  676 1208  857 1393  647  451  814 1188
Reordering of NBOs for storage:  1363  269 1408  507 1283 1253  744 1178 1353 1203
Reordering of NBOs for storage:  1009 1418  632  939  787  718  241  911 1368  256
Reordering of NBOs for storage:   577  940  745 1433  772 1238 1067 1378  366 1193
Reordering of NBOs for storage:  1079  912  424  633  801 1025 1388 1183  493 1403
Reordering of NBOs for storage:   536 1338 1323  997 1037  535 1010  240 1080  338
Reordering of NBOs for storage:  1398 1052 1278  773 1173 1039 1383  662 1443  604
Reordering of NBOs for storage:  1428  967  425  605  884 1358 1263 1051 1218  230
Reordering of NBOs for storage:   883  284  815 1024  968 1328 1248  983 1038 1448
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Reordering of NBOs for storage: 1313 1298 675 1066 661 996 1023 995 981 1065
Reordering of NBOs for storage: 452 283 522 982 1293 899 1373 927 508 1268
Reordering of NBOs for storage: 325 858 663 719 802 226 591 285 1233 634
Reordering of NBOs for storage: 620 941 494 913 257 732 746 953 869 453
Reordering of NBOs for storage: 800 523 557 578 396 340 382 871 777 590
Reordering of NBOs for storage: 356 1081 749 495 368 1413 703 255 480 648
Reordering of NBOs for storage: 774 369 1040 563 579 885 835 760 1101 1141
Reordering of NBOs for storage: 297 842 954 758 1011 730 466 897 618 717
Reordering of NBOs for storage: 1123 925 637 1136 1223 1163 870 1053 409 1110
Reordering of NBOs for storage: 969 1054 606 856 397 481 270 830 1096 467
Reordering of NBOs for storage: 1148 1150 305 955 902 828 827 689 623 688
Reordering of NBOs for storage: 310 383 311 549 696 1125 411 984 548 691
Reordering of NBOs for storage: 1108 1165 930 426 437 944 1343 242 506 1082
Reordering of NBOs for storage: 551 956 479 786 683 520 677 646 816 327
Reordering of NBOs for storage: 844 395 415 299 569 537 465 705 381 972
Reordering of NBOs for storage: 698 735 916 872 268 254 423 1012 799 431
Reordering of NBOs for storage: 565 1030 1026 341 320 763 716 492 998 339
Reordering of NBOs for storage: 702 855 660 576 282 324 888 357 841 674
Reordering of NBOs for storage: 813 609 296 562 534 484 367 314 754 833
Reordering of NBOs for storage: 485 438 271 593 594 971 788 421 353 318
Reordering of NBOs for storage: 1072 607 450 543 850 611 837 319 483 810
Reordering of NBOs for storage: 333 946 898 592 470 727 655 385 926 386
Reordering of NBOs for storage: 408 439 469 265 1068 399 440 708 886 988
Reordering of NBOs for storage: 435 739 442 401 821 1084 1316 731 471 759
Reordering of NBOs for storage: 1027 619 695 555 359 293 775 866 387 1069
Reordering of NBOs for storage: 665 1356 1013 641 355 792 915 1256 1436 974
Reordering of NBOs for storage: 400 936 649 259 742 1361 680 823 427 789
Reordering of NBOs for storage: 1251 793 570 1001 762 874 1164 734 1286 1094
Reordering of NBOs for storage: 958 1083 1109 848 1149 1281 1124 1311 595 443
Reordering of NBOs for storage: 1431 671 422 541 1236 1271 747 942 558 1139
Reordering of NBOs for storage: 531 313 1170 1130 441 352 304 1099 914 653
Reordering of NBOs for storage: 544 1058 635 1134 509 1056 804 1451 1155 1416
Reordering of NBOs for storage: 513 1306 1041 1376 354 1426 1411 1246 1115 1276
Reordering of NBOs for storage: 1231 622 574 1351 1366 737 525 236 1341 276
Reordering of NBOs for storage: 710 1241 629 1421 1391 1269 1301 336 901 275
Reordering of NBOs for storage: 713 1044 1371 1014 587 1449 1221 720 770 852
Reordering of NBOs for storage: 820 554 847 582 790 417 331 468 515 851
Reordering of NBOs for storage: 909 1045 482 1401 1216 288 1290 985 1000 624
Reordering of NBOs for storage: 258 1389 694 1396 552 929 1324 1326 714 765
Reordering of NBOs for storage: 302 234 943 819 1240 1299 229 1380 681 722
Reordering of NBOs for storage: 384 1098 1138 860 398 685 1370 330 447 934
Reordering of NBOs for storage: 524 1070 920 861 766 1304 932 1414 287 890
Reordering of NBOs for storage: 1381 1399 1429 1314 1249 1215 1160 476 512 1315
Reordering of NBOs for storage: 1420 1093 1219 1336 1133 803 1359 1244 1279 1289
Reordering of NBOs for storage: 1250 794 1335 1235 1285 1349 1360 1435 986 1055
Reordering of NBOs for storage: 1406 1274 1220 1430 1320 1355 1260 1305 1415 709
Reordering of NBOs for storage: 1234 1280 692 1104 1395 873 1424 322 711 316
Reordering of NBOs for storage: 1350 1245 1275 900 1339 1364 436 651 306 957
Reordering of NBOs for storage: 636 1425 1239 1374 761 1309 1229 1440 412 581
Reordering of NBOs for storage: 1375 1446 889 580 560 1409 277 1254 335 849
Reordering of NBOs for storage: 1369 1419 1259 1379 780 666 723 601 402 1400
Reordering of NBOs for storage: 1441 999 307 701 667 1346 568 805 1319 859
Reordering of NBOs for storage: 1439 598 678 1334 1386 1230 1224 488 1340 863
Reordering of NBOs for storage: 1295 904 627 959 428 621 791 1445 733 862
Reordering of NBOs for storage: 664 1344 1321 807 1365 566 1225 538 1410 1261
Reordering of NBOs for storage: 1266 1028 834 721 1310 289 1120 895 991 300
Reordering of NBOs for storage: 389 1450 928 1265 290 845 583 650 950 1394
Reordering of NBOs for storage: 328 1214 977 286 706 540 817 831 1385 1331
Reordering of NBOs for storage: 1291 1270 527 545 1255 363 764 668 1175 1296
Reordering of NBOs for storage: 1226 1195 776 652 1390 781 1210 358 1330 272
Reordering of NBOs for storage: 429 879 490 1300 514 1434 887 1354 1284 1144
Reordering of NBOs for storage: 274 614 1100 528 473 526 876 260 1205 907
Reordering of NBOs for storage: 1050 262 1145 906 806 596 1404 1325 1185 233
Reordering of NBOs for storage: 767 390 573 839 654 610 964 973 922 487
Reordering of NBOs for storage: 406 475 404 724 584 510 1405 597 1095 1200
Reordering of NBOs for storage: 1140 608 625 1135 1181 615 896 840 963 600
Reordering of NBOs for storage: 1018 935 796 877 273 261 279 918 628 903
Reordering of NBOs for storage: 1131 945 303 1190 1126 1166 1121 1116 684 1171
Reordering of NBOs for storage: 1106 1151 1156 1146 931 682 571 1191 750 1016
Reordering of NBOs for storage: 517 511 1111 586 736 1022 1161 626 1004 923
Reordering of NBOs for storage: 1119 784 1007 824 643 970 1180 227 1201 561

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 Reordering of NBOs for storage:  1086 1088  785 1105  905  572  317 1035 1345  542
 Reordering of NBOs for storage:   961 1062  979  738  539  656  880  748  700 1060
 Reordering of NBOs for storage:   960  875  756 1206  818  321  640  768  933 1159
 Reordering of NBOs for storage:   975  978 1211  924  753  332  878 1090 1186  391
 Reordering of NBOs for storage:   329  891 1209  779 1071  962  825 1085  757  292
 Reordering of NBOs for storage:  1042  752  639  952  822  864  893  638 1015  599
 Reordering of NBOs for storage:  1194  612 1029  919  740  751  434 1032 1129 1184
 Reordering of NBOs for storage:  1174 1196 1114  392 1204 1049 1169 1176 1154  669
 Reordering of NBOs for storage:   725  617  496  948  342 1091  235 1075  228 1003
 Reordering of NBOs for storage:  1076 1002  686  989  642  361 1074  976  454 1043
 Reordering of NBOs for storage:   644  613 1092  949  990  782  370  308  445 1031
 Reordering of NBOs for storage:  1057 1078  489  474  809 1020  697 1063  670  263
 Reordering of NBOs for storage:   741  334 1199  264  602  529 1073  679  994  546
 Reordering of NBOs for storage:   769  405  707  630  894  532 1017  585  658 1444
 Reordering of NBOs for storage:   987  280  726  446  518  501  344  498  266  712
 Reordering of NBOs for storage:  1033  553  778  808  459 1384  811  588  908  881
 Reordering of NBOs for storage:   418 1189  232  836  937  372  965  832  728 1264
 Reordering of NBOs for storage:   315  291  456  657  294  797  371 1329  846 1179
 Reordering of NBOs for storage:   672  362  993 1097  867  530 1005  865  567  556
 Reordering of NBOs for storage:  1034 1046 1006  301  343  497  237  516 1102  278
 Reordering of NBOs for storage:   693  448 1137 1087 1294  345 1047  853  795 1061
 Reordering of NBOs for storage:   414 1142  374  455 1019  364  503  500  457  462
 Reordering of NBOs for storage:   917  377  238 1059 1402  444 1252 1282 1222  486
 Reordering of NBOs for storage:   502 1227 1362  350 1232 1317 1432 1272 1342 1452
 Reordering of NBOs for storage:   403 1327 1302 1367 1277 1312  249 1307 1412 1237
 Reordering of NBOs for storage:  1352 1247 1427 1337 1357 1257 1287 1437 1322 1377
 Reordering of NBOs for storage:  1447 1217  375 1122 1372 1417 1382 1242 1397 1422
 Reordering of NBOs for storage:  1132 1392 1162 1172 1442 1292 1107 1262  252 1157
 Reordering of NBOs for storage:  1407 1147 1117 1332 1267  460 1297 1127 1387 1347
 Reordering of NBOs for storage:  1167 1152 1112  378  349  388  461  472  376 1202
 Reordering of NBOs for storage:   420  504 1207 1192 1212 1182  348 1187 1197 1177
 Reordering of NBOs for storage:   947  250  245  346  360  247  432  347  251  373
 Reordering of NBOs for storage:   246  413  458  499  433  248  419  244  416  430
 Reordering of NBOs for storage:   951  783  921  645  239  755  449  365 1021  616
 Reordering of NBOs for storage:  1089  980  892 1064 1048 1036  992 1077 1008  882
 Reordering of NBOs for storage:   966  826  547  687  603  854  309  337  575  938
 Reordering of NBOs for storage:   715  559  673  743  910  533  631  295  519  838
 Reordering of NBOs for storage:   729  771  323  868  393  477  699  407  589  812
 Reordering of NBOs for storage:   267  491  798  281  659  351  505  463  379  253
 Labels of output orbitals:  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR
CR  CR  CR
 Labels of output orbitals:  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR
CR  CR  CR
 Labels of output orbitals:  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR  CR
CR  CR  CR
 Labels of output orbitals:  CR  CR  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD
BD  BD  BD
 Labels of output orbitals:  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD
BD  BD  LP
 Labels of output orbitals:  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD
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 Labels of output orbitals:  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD
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 Labels of output orbitals:  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD
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 Labels of output orbitals:  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD
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 Labels of output orbitals:  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD  BD
BD  BD  BD
 Labels of output orbitals:  BD  BD  BD  BD  BD  BD  BD  LP  BD  BD  BD  BD  BD  BD  BD  BD  BD
BD  BD  BD
 Labels of output orbitals:  BD  BD  LP  LP  BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD*
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 Labels of output orbitals:  LP* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD*
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Labels of output orbitals: BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD*
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Labels of output orbitals: BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD*
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Labels of output orbitals: BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD* BD*
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Labels of output orbitals: BD* BD* BD* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
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RY* RY* RY*
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RY* RY* RY*
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RY* RY* RY*
Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
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RY* RY* RY*
Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
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RY* RY* RY*
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RY* RY* RY*
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RY* RY* RY*
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RY* RY* RY*
Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
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RY* RY* RY*
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RY* RY* RY*
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Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
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RY* RY* RY*
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RY* RY* RY*
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RY* RY* RY*
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Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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Labels of output orbitals: RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*

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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
RY* RY* RY*
 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
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 Labels of output orbitals:  RY* RY* RY* RY* RY* RY* RY* RY* RY* RY*
 1\1\GINC-NODE001\SP\RPBEPBE\TZVP\C55H72B2N4O1\VANKA\14-Jun-2015\0\\# p
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29,-0.256053,4.554723\H,0,4.276453,4.166041,5.690685\H,0,9.480558,2.75
4655,2.902624\H,0,9.516569,3.137737,7.680761\H,0,9.385503,0.183492,2.9
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0,7.609478,0.247324,1.267367\H,0,6.857098,-1.214117,1.946314\H,0,6.893
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@

"TIGER, TIGER BURNING BRIGHT
IN THE FOREST OF THE NIGHT.
WHAT IMMORTAL HAND OR EYE
CAN FRAME THY FEARFUL SYMMETRYE?"
- WILLIAM BLAKE

Job cpu time: 1 days 9 hours 17 minutes 12.0 seconds.
File lengths (MBytes): RWF= 1383 Int= 0 D2E= 0 Chk= 90 Scr= 1
Normal termination of Gaussian 09 at Sun Jun 14 03:36:36 2015.