

\*\*\*\*\*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: 579472 in NPA, 769865 in NBO, 578878 in NLMO ( 33551006 available)

NATURAL POPULATIONS: Natural atomic orbital occupancies

NAO	Atom	No	lang	Type(AO)	Occupancy	Energy
1	N	1	S	Cor( 1S)	1.99944	-13.87358
2	N	1	S	Val( 2S)	1.20026	-0.52994
3	N	1	S	Ryd( 3S)	0.00145	1.33972
4	N	1	S	Ryd( 4S)	0.00016	2.88617
5	N	1	S	Ryd( 5S)	0.00000	30.13441
6	N	1	px	Val( 2p)	1.25936	-0.24080
7	N	1	px	Ryd( 3p)	0.00205	1.11294
8	N	1	px	Ryd( 4p)	0.00024	2.40468
9	N	1	py	Val( 2p)	1.30911	-0.24469
10	N	1	py	Ryd( 3p)	0.00323	1.08639
11	N	1	py	Ryd( 4p)	0.00027	2.37027
12	N	1	pz	Val( 2p)	1.49074	-0.24322
13	N	1	pz	Ryd( 3p)	0.00247	0.62485
14	N	1	pz	Ryd( 4p)	0.00026	2.06920
15	N	1	dxy	Ryd( 3d)	0.00092	2.69512
16	N	1	dxz	Ryd( 3d)	0.00055	2.29593
17	N	1	dyz	Ryd( 3d)	0.00069	2.47106
18	N	1	dx2y2	Ryd( 3d)	0.00120	2.81967
19	N	1	dz2	Ryd( 3d)	0.00056	2.57384
20	C	2	S	Cor( 1S)	1.99878	-9.79480
21	C	2	S	Val( 2S)	0.94267	-0.19996
22	C	2	S	Ryd( 4S)	0.00312	1.38072
23	C	2	S	Ryd( 3S)	0.00021	1.22220
24	C	2	S	Ryd( 5S)	0.00000	21.37289
25	C	2	px	Val( 2p)	1.10405	-0.07199
26	C	2	px	Ryd( 4p)	0.00597	1.63024
27	C	2	px	Ryd( 3p)	0.00084	1.10441
28	C	2	py	Val( 2p)	0.80996	-0.04926
29	C	2	py	Ryd( 4p)	0.00279	1.32358
30	C	2	py	Ryd( 3p)	0.00104	1.20057
31	C	2	pz	Val( 2p)	0.91807	-0.11113
32	C	2	pz	Ryd( 4p)	0.00203	1.00213
33	C	2	pz	Ryd( 3p)	0.00038	0.97603
34	C	2	dxy	Ryd( 3d)	0.00098	2.62001
35	C	2	dxz	Ryd( 3d)	0.00104	2.00090
36	C	2	dyz	Ryd( 3d)	0.00066	2.08899
37	C	2	dx2y2	Ryd( 3d)	0.00074	2.51982
38	C	2	dz2	Ryd( 3d)	0.00050	2.25828
39	N	3	S	Cor( 1S)	1.99944	-13.87211
40	N	3	S	Val( 2S)	1.20362	-0.52785
41	N	3	S	Ryd( 3S)	0.00127	1.37292
42	N	3	S	Ryd( 4S)	0.00017	2.96280
43	N	3	S	Ryd( 5S)	0.00000	30.01445
44	N	3	px	Val( 2p)	1.26928	-0.23805
45	N	3	px	Ryd( 3p)	0.00205	0.91261
46	N	3	px	Ryd( 4p)	0.00017	2.43013
47	N	3	py	Val( 2p)	1.29911	-0.24109
48	N	3	py	Ryd( 3p)	0.00331	1.26533
49	N	3	py	Ryd( 4p)	0.00032	2.31862
50	N	3	pz	Val( 2p)	1.48310	-0.24060

51	N	3	pz	Ryd( 3p)	0.00240	0.66589
52	N	3	pz	Ryd( 4p)	0.00026	2.05998
53	N	3	dxz	Ryd( 3d)	0.00127	2.83524
54	N	3	dxz	Ryd( 3d)	0.00064	2.30445
55	N	3	dyz	Ryd( 3d)	0.00063	2.45341
56	N	3	dx2y2	Ryd( 3d)	0.00085	2.69135
57	N	3	dz2	Ryd( 3d)	0.00055	2.57903
58	C	4	S	Cor( 1S)	1.99911	-9.79234
59	C	4	S	Val( 2S)	0.95582	-0.23420
60	C	4	S	Ryd( 3S)	0.00099	0.88767
61	C	4	S	Ryd( 4S)	0.00007	1.11360
62	C	4	S	Ryd( 5S)	0.00001	21.33693
63	C	4	px	Val( 2p)	1.04669	-0.07824
64	C	4	px	Ryd( 3p)	0.00199	0.99856
65	C	4	px	Ryd( 4p)	0.00076	1.54980
66	C	4	py	Val( 2p)	1.00679	-0.10050
67	C	4	py	Ryd( 3p)	0.00389	0.81374
68	C	4	py	Ryd( 4p)	0.00046	1.28279
69	C	4	pz	Val( 2p)	1.06460	-0.14047
70	C	4	pz	Ryd( 3p)	0.00418	0.48648
71	C	4	pz	Ryd( 4p)	0.00046	1.20660
72	C	4	dxz	Ryd( 3d)	0.00088	2.54615
73	C	4	dxz	Ryd( 3d)	0.00069	1.95250
74	C	4	dyz	Ryd( 3d)	0.00054	2.07631
75	C	4	dx2y2	Ryd( 3d)	0.00066	2.48141
76	C	4	dz2	Ryd( 3d)	0.00054	2.22600
77	C	5	S	Cor( 1S)	1.99911	-9.79324
78	C	5	S	Val( 2S)	0.95630	-0.23513
79	C	5	S	Ryd( 3S)	0.00099	0.88082
80	C	5	S	Ryd( 4S)	0.00007	1.11351
81	C	5	S	Ryd( 5S)	0.00001	21.33334
82	C	5	px	Val( 2p)	0.89172	-0.07800
83	C	5	px	Ryd( 3p)	0.00279	0.80803
84	C	5	px	Ryd( 4p)	0.00052	1.28648
85	C	5	py	Val( 2p)	1.13537	-0.10246
86	C	5	py	Ryd( 3p)	0.00319	0.96559
87	C	5	py	Ryd( 4p)	0.00069	1.49429
88	C	5	pz	Val( 2p)	1.09550	-0.14155
89	C	5	pz	Ryd( 3p)	0.00411	0.51505
90	C	5	pz	Ryd( 4p)	0.00050	1.24878
91	C	5	dxz	Ryd( 3d)	0.00063	2.40729
92	C	5	dxz	Ryd( 3d)	0.00078	1.92449
93	C	5	dyz	Ryd( 3d)	0.00053	2.11552
94	C	5	dx2y2	Ryd( 3d)	0.00089	2.60709
95	C	5	dz2	Ryd( 3d)	0.00046	2.22657
96	B	6	S	Cor( 1S)	1.99707	-6.29777
97	B	6	S	Val( 2S)	0.62756	0.11896
98	B	6	S	Ryd( 4S)	0.00203	2.83854
99	B	6	S	Ryd( 3S)	0.00029	2.63925
100	B	6	S	Ryd( 5S)	0.00006	11.48960
101	B	6	px	Val( 2p)	0.87525	0.12408
102	B	6	px	Ryd( 4p)	0.00259	1.06997
103	B	6	px	Ryd( 3p)	0.00089	1.00077
104	B	6	py	Val( 2p)	0.91541	0.08334
105	B	6	py	Ryd( 4p)	0.00120	0.92352
106	B	6	py	Ryd( 3p)	0.00068	0.70363
107	B	6	pz	Val( 2p)	0.77832	0.03607
108	B	6	pz	Ryd( 4p)	0.00065	0.76662
109	B	6	pz	Ryd( 3p)	0.00032	0.58062
110	B	6	dxz	Ryd( 3d)	0.00072	2.00001
111	B	6	dxz	Ryd( 3d)	0.00054	1.63090
112	B	6	dyz	Ryd( 3d)	0.00037	1.39057
113	B	6	dx2y2	Ryd( 3d)	0.00078	2.23239
114	B	6	dz2	Ryd( 3d)	0.00033	1.72147
115	C	7	S	Cor( 1S)	1.99860	-9.72863
116	C	7	S	Val( 2S)	0.90122	-0.13899
117	C	7	S	Ryd( 4S)	0.00946	1.42193

118	C	7	S	Ryd( 3S)	0.00018	1.10222
119	C	7	S	Ryd( 5S)	0.00000	21.44259
120	C	7	px	Val( 2p)	1.18523	-0.02076
121	C	7	px	Ryd( 3p)	0.00102	1.00752
122	C	7	px	Ryd( 4p)	0.00012	1.30872
123	C	7	py	Val( 2p)	0.88707	0.00635
124	C	7	py	Ryd( 3p)	0.01433	1.02692
125	C	7	py	Ryd( 4p)	0.00027	1.42994
126	C	7	pz	Val( 2p)	0.87788	-0.04749
127	C	7	pz	Ryd( 3p)	0.00130	0.70015
128	C	7	pz	Ryd( 4p)	0.00036	1.30027
129	C	7	dxz	Ryd( 3d)	0.00221	2.50338
130	C	7	dxz	Ryd( 3d)	0.00022	1.89929
131	C	7	dyz	Ryd( 3d)	0.00236	2.24656
132	C	7	dx2y2	Ryd( 3d)	0.00127	2.50226
133	C	7	dz2	Ryd( 3d)	0.00077	2.18972
134	O	8	S	Cor( 1S)	1.99982	-18.39696
135	O	8	S	Val( 2S)	1.70220	-0.75580
136	O	8	S	Ryd( 3S)	0.00233	1.24534
137	O	8	S	Ryd( 4S)	0.00009	5.42551
138	O	8	S	Ryd( 5S)	0.00000	40.95942
139	O	8	px	Val( 2p)	1.76758	-0.14320
140	O	8	px	Ryd( 3p)	0.00564	0.73503
141	O	8	px	Ryd( 4p)	0.00003	2.72699
142	O	8	py	Val( 2p)	1.55254	-0.18884
143	O	8	py	Ryd( 3p)	0.00213	0.56200
144	O	8	py	Ryd( 4p)	0.00013	3.00737
145	O	8	pz	Val( 2p)	1.55941	-0.15273
146	O	8	pz	Ryd( 3p)	0.00276	0.64972
147	O	8	pz	Ryd( 4p)	0.00002	2.66997
148	O	8	dxz	Ryd( 3d)	0.00120	2.92505
149	O	8	dxz	Ryd( 3d)	0.00013	2.66076
150	O	8	dyz	Ryd( 3d)	0.00142	2.94203
151	O	8	dx2y2	Ryd( 3d)	0.00147	3.18364
152	O	8	dz2	Ryd( 3d)	0.00059	2.81520
153	C	9	S	Cor( 1S)	1.99932	-9.78455
154	C	9	S	Val( 2S)	1.10312	-0.28727
155	C	9	S	Ryd( 3S)	0.00093	1.01370
156	C	9	S	Ryd( 4S)	0.00007	1.89936
157	C	9	S	Ryd( 5S)	0.00000	21.15771
158	C	9	px	Val( 2p)	1.28337	-0.11787
159	C	9	px	Ryd( 3p)	0.00176	0.61160
160	C	9	px	Ryd( 4p)	0.00021	1.40492
161	C	9	py	Val( 2p)	0.89042	-0.10041
162	C	9	py	Ryd( 3p)	0.00191	0.56666
163	C	9	py	Ryd( 4p)	0.00038	1.27582
164	C	9	pz	Val( 2p)	1.16548	-0.11130
165	C	9	pz	Ryd( 3p)	0.00108	0.57435
166	C	9	pz	Ryd( 4p)	0.00018	1.39805
167	C	9	dxz	Ryd( 3d)	0.00032	2.22967
168	C	9	dxz	Ryd( 3d)	0.00050	2.29989
169	C	9	dyz	Ryd( 3d)	0.00070	2.32457
170	C	9	dx2y2	Ryd( 3d)	0.00085	2.52806
171	C	9	dz2	Ryd( 3d)	0.00056	2.31003
172	C	10	S	Cor( 1S)	1.99933	-9.79463
173	C	10	S	Val( 2S)	1.09983	-0.29734
174	C	10	S	Ryd( 3S)	0.00099	0.94776
175	C	10	S	Ryd( 4S)	0.00008	1.77555
176	C	10	S	Ryd( 5S)	0.00000	21.25560
177	C	10	px	Val( 2p)	1.13468	-0.12383
178	C	10	px	Ryd( 3p)	0.00164	0.54358
179	C	10	px	Ryd( 4p)	0.00025	1.34653
180	C	10	py	Val( 2p)	1.01634	-0.11534
181	C	10	py	Ryd( 3p)	0.00110	0.51972
182	C	10	py	Ryd( 4p)	0.00036	1.31496
183	C	10	pz	Val( 2p)	1.18931	-0.12228
184	C	10	pz	Ryd( 3p)	0.00156	0.54183
185	C	10	pz	Ryd( 4p)	0.00019	1.42235

186	C	10	dxy	Ryd( 3d)	0.00073	2.45143
187	C	10	dxz	Ryd( 3d)	0.00038	2.04124
188	C	10	dyz	Ryd( 3d)	0.00069	2.36919
189	C	10	dx2y2	Ryd( 3d)	0.00050	2.33626
190	C	10	dz2	Ryd( 3d)	0.00068	2.44832
191	B	11	S	Cor( 1S)	1.99781	-6.30802
192	B	11	S	Val( 2S)	0.66143	0.07761
193	B	11	S	Ryd( 4S)	0.00179	3.26121
194	B	11	S	Ryd( 3S)	0.00075	1.57863
195	B	11	S	Ryd( 5S)	0.00012	6.53467
196	B	11	px	Val( 2p)	0.84312	0.16035
197	B	11	px	Ryd( 3p)	0.00270	0.85260
198	B	11	px	Ryd( 4p)	0.00113	1.38627
199	B	11	py	Val( 2p)	0.85959	0.06974
200	B	11	py	Ryd( 3p)	0.00180	0.76937
201	B	11	py	Ryd( 4p)	0.00065	0.97657
202	B	11	pz	Val( 2p)	0.65279	0.03030
203	B	11	pz	Ryd( 3p)	0.00124	0.55078
204	B	11	pz	Ryd( 4p)	0.00049	0.82963
205	B	11	dxy	Ryd( 3d)	0.00077	1.82350
206	B	11	dxz	Ryd( 3d)	0.00058	1.66332
207	B	11	dyz	Ryd( 3d)	0.00049	1.41225
208	B	11	dx2y2	Ryd( 3d)	0.00057	2.19814
209	B	11	dz2	Ryd( 3d)	0.00049	1.65423
210	C	12	S	Cor( 1S)	1.99873	-9.77950
211	C	12	S	Val( 2S)	0.94419	-0.19036
212	C	12	S	Ryd( 3S)	0.00306	1.39680
213	C	12	S	Ryd( 4S)	0.00064	1.44270
214	C	12	S	Ryd( 5S)	0.00000	21.36372
215	C	12	px	Val( 2p)	1.14550	-0.07419
216	C	12	px	Ryd( 4p)	0.00605	1.68769
217	C	12	px	Ryd( 3p)	0.00054	1.11517
218	C	12	py	Val( 2p)	0.87512	-0.06100
219	C	12	py	Ryd( 4p)	0.00216	1.18800
220	C	12	py	Ryd( 3p)	0.00098	1.09447
221	C	12	pz	Val( 2p)	0.89176	-0.07539
222	C	12	pz	Ryd( 4p)	0.00201	1.09422
223	C	12	pz	Ryd( 3p)	0.00080	1.04713
224	C	12	dxy	Ryd( 3d)	0.00115	2.46372
225	C	12	dxz	Ryd( 3d)	0.00100	2.32973
226	C	12	dyz	Ryd( 3d)	0.00046	2.40791
227	C	12	dx2y2	Ryd( 3d)	0.00067	2.35414
228	C	12	dz2	Ryd( 3d)	0.00067	2.03235
229	N	13	S	Cor( 1S)	1.99946	-13.85323
230	N	13	S	Val( 2S)	1.19631	-0.50907
231	N	13	S	Ryd( 3S)	0.00149	1.45519
232	N	13	S	Ryd( 4S)	0.00020	2.82182
233	N	13	S	Ryd( 5S)	0.00000	30.11221
234	N	13	px	Val( 2p)	1.26050	-0.22067
235	N	13	px	Ryd( 3p)	0.00186	0.95867
236	N	13	px	Ryd( 4p)	0.00020	2.39314
237	N	13	py	Val( 2p)	1.37259	-0.22285
238	N	13	py	Ryd( 3p)	0.00338	1.05770
239	N	13	py	Ryd( 4p)	0.00034	2.25968
240	N	13	pz	Val( 2p)	1.44259	-0.22213
241	N	13	pz	Ryd( 3p)	0.00358	0.87015
242	N	13	pz	Ryd( 4p)	0.00035	2.18671
243	N	13	dxy	Ryd( 3d)	0.00101	2.62262
244	N	13	dxz	Ryd( 3d)	0.00079	2.50717
245	N	13	dyz	Ryd( 3d)	0.00067	2.75487
246	N	13	dx2y2	Ryd( 3d)	0.00074	2.65274
247	N	13	dz2	Ryd( 3d)	0.00063	2.40066
248	C	14	S	Cor( 1S)	1.99910	-9.77552
249	C	14	S	Val( 2S)	0.95276	-0.21635
250	C	14	S	Ryd( 3S)	0.00102	0.89954
251	C	14	S	Ryd( 4S)	0.00007	1.09222
252	C	14	S	Ryd( 5S)	0.00001	21.38179

253	C	14	px	Val( 2p)	0.96572	-0.05924
254	C	14	px	Ryd( 3p)	0.00228	0.91835
255	C	14	px	Ryd( 4p)	0.00063	1.46000
256	C	14	py	Val( 2p)	1.06465	-0.10141
257	C	14	py	Ryd( 3p)	0.00423	0.71904
258	C	14	py	Ryd( 4p)	0.00052	1.28583
259	C	14	pz	Val( 2p)	1.09540	-0.10785
260	C	14	pz	Ryd( 3p)	0.00378	0.68400
261	C	14	pz	Ryd( 4p)	0.00049	1.34003
262	C	14	dxy	Ryd( 3d)	0.00074	2.26933
263	C	14	dxz	Ryd( 3d)	0.00082	2.16828
264	C	14	dyz	Ryd( 3d)	0.00059	2.43991
265	C	14	dx2y2	Ryd( 3d)	0.00072	2.42302
266	C	14	dz2	Ryd( 3d)	0.00054	2.07135
267	C	15	S	Cor( 1S)	1.99910	-9.77494
268	C	15	S	Val( 2S)	0.95269	-0.21708
269	C	15	S	Ryd( 3S)	0.00100	0.87782
270	C	15	S	Ryd( 4S)	0.00007	1.10411
271	C	15	S	Ryd( 5S)	0.00001	21.37219
272	C	15	px	Val( 2p)	0.94576	-0.05952
273	C	15	px	Ryd( 3p)	0.00239	0.87237
274	C	15	px	Ryd( 4p)	0.00066	1.45127
275	C	15	py	Val( 2p)	1.11245	-0.10261
276	C	15	py	Ryd( 3p)	0.00438	0.72644
277	C	15	py	Ryd( 4p)	0.00060	1.37462
278	C	15	pz	Val( 2p)	1.08430	-0.10835
279	C	15	pz	Ryd( 3p)	0.00431	0.63998
280	C	15	pz	Ryd( 4p)	0.00048	1.34403
281	C	15	dxy	Ryd( 3d)	0.00075	2.22948
282	C	15	dxz	Ryd( 3d)	0.00073	2.16721
283	C	15	dyz	Ryd( 3d)	0.00060	2.44948
284	C	15	dx2y2	Ryd( 3d)	0.00069	2.45447
285	C	15	dz2	Ryd( 3d)	0.00056	2.06636
286	N	16	S	Cor( 1S)	1.99946	-13.85576
287	N	16	S	Val( 2S)	1.19633	-0.51187
288	N	16	S	Ryd( 3S)	0.00118	1.50907
289	N	16	S	Ryd( 4S)	0.00018	2.71650
290	N	16	S	Ryd( 5S)	0.00000	30.11678
291	N	16	px	Val( 2p)	1.26219	-0.22286
292	N	16	px	Ryd( 3p)	0.00198	0.98426
293	N	16	px	Ryd( 4p)	0.00019	2.35214
294	N	16	py	Val( 2p)	1.39380	-0.22542
295	N	16	py	Ryd( 3p)	0.00321	0.93970
296	N	16	py	Ryd( 4p)	0.00037	2.24720
297	N	16	pz	Val( 2p)	1.42402	-0.22452
298	N	16	pz	Ryd( 3p)	0.00339	0.93423
299	N	16	pz	Ryd( 4p)	0.00038	2.21135
300	N	16	dxy	Ryd( 3d)	0.00085	2.56951
301	N	16	dxz	Ryd( 3d)	0.00078	2.51701
302	N	16	dyz	Ryd( 3d)	0.00067	2.77732
303	N	16	dx2y2	Ryd( 3d)	0.00087	2.64224
304	N	16	dz2	Ryd( 3d)	0.00063	2.41456
305	C	17	S	Cor( 1S)	1.99933	-9.77872
306	C	17	S	Val( 2S)	1.09804	-0.27956
307	C	17	S	Ryd( 3S)	0.00102	0.97653
308	C	17	S	Ryd( 4S)	0.00005	2.19158
309	C	17	S	Ryd( 5S)	0.00000	20.79107
310	C	17	px	Val( 2p)	1.21057	-0.10684
311	C	17	px	Ryd( 3p)	0.00153	0.67014
312	C	17	px	Ryd( 4p)	0.00022	1.49458
313	C	17	py	Val( 2p)	1.00761	-0.09814
314	C	17	py	Ryd( 3p)	0.00125	0.60575
315	C	17	py	Ryd( 4p)	0.00034	1.31414
316	C	17	pz	Val( 2p)	1.11574	-0.10227
317	C	17	pz	Ryd( 3p)	0.00122	0.54002
318	C	17	pz	Ryd( 4p)	0.00024	1.31061
319	C	17	dxy	Ryd( 3d)	0.00064	2.50816
320	C	17	dxz	Ryd( 3d)	0.00059	2.35647

321	C	17	dyz	Ryd( 3d)	0.00072	2.48073
322	C	17	dx2y2	Ryd( 3d)	0.00044	2.16005
323	C	17	dz2	Ryd( 3d)	0.00063	2.22663
324	C	18	S	Cor( 1S)	1.99934	-9.78803
325	C	18	S	Val( 2S)	1.09446	-0.28798
326	C	18	S	Ryd( 3S)	0.00096	0.91915
327	C	18	S	Ryd( 4S)	0.00009	1.72200
328	C	18	S	Ryd( 5S)	0.00000	21.26110
329	C	18	px	Val( 2p)	1.20108	-0.11828
330	C	18	px	Ryd( 3p)	0.00160	0.54505
331	C	18	px	Ryd( 4p)	0.00022	1.45412
332	C	18	py	Val( 2p)	1.06769	-0.10932
333	C	18	py	Ryd( 3p)	0.00121	0.56356
334	C	18	py	Ryd( 4p)	0.00035	1.42735
335	C	18	pz	Val( 2p)	1.06509	-0.10832
336	C	18	pz	Ryd( 3p)	0.00126	0.50369
337	C	18	pz	Ryd( 4p)	0.00030	1.33400
338	C	18	dxz	Ryd( 3d)	0.00050	2.28218
339	C	18	dxz	Ryd( 3d)	0.00035	2.19090
340	C	18	dyz	Ryd( 3d)	0.00063	2.45835
341	C	18	dx2y2	Ryd( 3d)	0.00058	2.36393
342	C	18	dz2	Ryd( 3d)	0.00097	2.38900
343	H	19	S	Val( 1S)	0.76643	-0.01400
344	H	19	S	Ryd( 3S)	0.00032	1.41083
345	H	19	S	Ryd( 2S)	0.00017	0.86360
346	H	19	px	Ryd( 2p)	0.00047	2.60775
347	H	19	py	Ryd( 2p)	0.00023	1.99193
348	H	19	pz	Ryd( 2p)	0.00026	1.61605
349	H	20	S	Val( 1S)	0.76796	-0.01622
350	H	20	S	Ryd( 2S)	0.00046	0.87317
351	H	20	S	Ryd( 3S)	0.00020	1.39330
352	H	20	px	Ryd( 2p)	0.00027	2.14688
353	H	20	py	Ryd( 2p)	0.00040	2.37019
354	H	20	pz	Ryd( 2p)	0.00030	1.69280
355	H	21	S	Val( 1S)	0.77074	-0.00043
356	H	21	S	Ryd( 3S)	0.00035	1.27082
357	H	21	S	Ryd( 2S)	0.00017	1.02631
358	H	21	px	Ryd( 2p)	0.00040	2.42632
359	H	21	py	Ryd( 2p)	0.00028	1.91206
360	H	21	pz	Ryd( 2p)	0.00032	1.92450
361	H	22	S	Val( 1S)	0.77106	-0.00125
362	H	22	S	Ryd( 3S)	0.00033	1.36636
363	H	22	S	Ryd( 2S)	0.00017	0.92068
364	H	22	px	Ryd( 2p)	0.00038	2.37129
365	H	22	py	Ryd( 2p)	0.00033	2.01806
366	H	22	pz	Ryd( 2p)	0.00030	1.86808
367	H	23	S	Val( 1S)	0.78704	-0.00481
368	H	23	S	Ryd( 2S)	0.00045	0.63272
369	H	23	S	Ryd( 3S)	0.00013	1.76491
370	H	23	px	Ryd( 2p)	0.00031	2.30024
371	H	23	py	Ryd( 2p)	0.00032	2.03701
372	H	23	pz	Ryd( 2p)	0.00018	1.81299
373	H	24	S	Val( 1S)	0.79078	0.00113
374	H	24	S	Ryd( 2S)	0.00125	0.66030
375	H	24	S	Ryd( 3S)	0.00015	1.77590
376	H	24	px	Ryd( 2p)	0.00018	1.95053
377	H	24	py	Ryd( 2p)	0.00028	1.81789
378	H	24	pz	Ryd( 2p)	0.00032	2.43565
379	H	25	S	Val( 1S)	0.73307	0.03867
380	H	25	S	Ryd( 2S)	0.00178	0.76647
381	H	25	S	Ryd( 3S)	0.00025	1.87911
382	H	25	px	Ryd( 2p)	0.00030	2.19501
383	H	25	py	Ryd( 2p)	0.00025	2.02520

384	H	25	pz	Ryd( 2p)	0.00029	2.01868
385	H	26	S	Val( 1S)	0.79029	-0.01397
386	H	26	S	Ryd( 2S)	0.00078	0.61008
387	H	26	S	Ryd( 3S)	0.00014	1.76150
388	H	26	px	Ryd( 2p)	0.00022	1.91092
389	H	26	py	Ryd( 2p)	0.00041	2.39681
390	H	26	pz	Ryd( 2p)	0.00017	1.80170
391	H	27	S	Val( 1S)	0.78639	-0.00490
392	H	27	S	Ryd( 2S)	0.00123	0.64435
393	H	27	S	Ryd( 3S)	0.00014	1.75944
394	H	27	px	Ryd( 2p)	0.00017	1.78962
395	H	27	py	Ryd( 2p)	0.00027	1.85645
396	H	27	pz	Ryd( 2p)	0.00033	2.51143
397	H	28	S	Val( 1S)	0.75302	0.01225
398	H	28	S	Ryd( 2S)	0.00078	1.08639
399	H	28	S	Ryd( 3S)	0.00015	1.63479
400	H	28	px	Ryd( 2p)	0.00040	2.59581
401	H	28	py	Ryd( 2p)	0.00019	1.76913
402	H	28	pz	Ryd( 2p)	0.00017	1.81987
403	H	29	S	Val( 1S)	0.78634	-0.01911
404	H	29	S	Ryd( 2S)	0.00070	0.66884
405	H	29	S	Ryd( 3S)	0.00013	1.69434
406	H	29	px	Ryd( 2p)	0.00020	1.73161
407	H	29	py	Ryd( 2p)	0.00020	1.85282
408	H	29	pz	Ryd( 2p)	0.00038	2.52032
409	H	30	S	Val( 1S)	0.72573	0.02502
410	H	30	S	Ryd( 2S)	0.00066	1.17417
411	H	30	S	Ryd( 3S)	0.00018	1.73633
412	H	30	px	Ryd( 2p)	0.00033	2.58558
413	H	30	py	Ryd( 2p)	0.00028	1.87647
414	H	30	pz	Ryd( 2p)	0.00013	1.76125
415	H	31	S	Val( 1S)	0.78821	-0.01980
416	H	31	S	Ryd( 2S)	0.00078	0.64618
417	H	31	S	Ryd( 3S)	0.00013	1.71632
418	H	31	px	Ryd( 2p)	0.00021	1.73965
419	H	31	py	Ryd( 2p)	0.00033	2.29308
420	H	31	pz	Ryd( 2p)	0.00026	2.07297
421	H	32	S	Val( 1S)	0.78674	-0.00967
422	H	32	S	Ryd( 2S)	0.00056	0.70064
423	H	32	S	Ryd( 3S)	0.00014	1.68526
424	H	32	px	Ryd( 2p)	0.00019	1.94107
425	H	32	py	Ryd( 2p)	0.00033	2.07337
426	H	32	pz	Ryd( 2p)	0.00028	2.13053
427	H	33	S	Val( 1S)	0.78690	-0.00921
428	H	33	S	Ryd( 2S)	0.00062	0.71236
429	H	33	S	Ryd( 3S)	0.00014	1.68188
430	H	33	px	Ryd( 2p)	0.00020	1.97033
431	H	33	py	Ryd( 2p)	0.00025	1.75269
432	H	33	pz	Ryd( 2p)	0.00035	2.42243
433	H	34	S	Val( 1S)	0.70985	0.05033
434	H	34	S	Ryd( 2S)	0.00205	0.87294
435	H	34	S	Ryd( 3S)	0.00030	1.91652
436	H	34	px	Ryd( 2p)	0.00050	2.59304
437	H	34	py	Ryd( 2p)	0.00026	1.89430
438	H	34	pz	Ryd( 2p)	0.00011	1.78731

WARNING: 1 low occupancy (<1.9990e) core orbital found on C 2  
1 low occupancy (<1.9990e) core orbital found on B 6  
1 low occupancy (<1.9990e) core orbital found on C 7  
1 low occupancy (<1.9990e) core orbital found on B 11  
1 low occupancy (<1.9990e) core orbital found on C 12

WARNING: Population inversion found on atom C 2  
 Population inversion found on atom B 6  
 Population inversion found on atom C 7  
 Population inversion found on atom B 11  
 Population inversion found on atom C 12  
 Population inversion found on atom H 19  
 Population inversion found on atom H 21  
 Population inversion found on atom H 22

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
N	1	-0.27296	1.99944	5.25947	0.01404	7.27296
C	2	0.20616	1.99878	3.77475	0.02030	5.79384
N	3	-0.26843	1.99944	5.25511	0.01388	7.26843
C	4	-0.08914	1.99911	4.07390	0.01612	6.08914
C	5	-0.09415	1.99911	4.07888	0.01616	6.09415
B	6	-0.20507	1.99707	3.19654	0.01146	5.20507
C	7	0.11614	1.99860	3.85140	0.03386	5.88386
O	8	-0.59949	1.99982	6.58172	0.01794	8.59949
C	9	-0.45114	1.99932	4.44239	0.00943	6.45114
C	10	-0.44866	1.99933	4.44016	0.00916	6.44866
B	11	-0.02830	1.99781	3.01693	0.01356	5.02830
C	12	0.12451	1.99873	3.85657	0.02019	5.87549
N	13	-0.28669	1.99946	5.27199	0.01525	7.28669
C	14	-0.09407	1.99910	4.07854	0.01643	6.09407
C	15	-0.11152	1.99910	4.09520	0.01722	6.11152
N	16	-0.29049	1.99946	5.27635	0.01468	7.29049
C	17	-0.44018	1.99933	4.43196	0.00889	6.44018
C	18	-0.43670	1.99934	4.42832	0.00903	6.43670
H	19	0.23212	0.00000	0.76643	0.00145	0.76788
H	20	0.23041	0.00000	0.76796	0.00164	0.76959
H	21	0.22773	0.00000	0.77074	0.00152	0.77227
H	22	0.22744	0.00000	0.77106	0.00150	0.77256
H	23	0.21156	0.00000	0.78704	0.00139	0.78844
H	24	0.20702	0.00000	0.79078	0.00220	0.79298
H	25	0.26406	0.00000	0.73307	0.00287	0.73594
H	26	0.20799	0.00000	0.79029	0.00172	0.79201
H	27	0.21148	0.00000	0.78639	0.00213	0.78852
H	28	0.24529	0.00000	0.75302	0.00169	0.75471
H	29	0.21205	0.00000	0.78634	0.00161	0.78795
H	30	0.27269	0.00000	0.72573	0.00158	0.72731
H	31	0.21008	0.00000	0.78821	0.00171	0.78992
H	32	0.21176	0.00000	0.78674	0.00149	0.78824
H	33	0.21155	0.00000	0.78690	0.00155	0.78845
H	34	0.28694	0.00000	0.70985	0.00321	0.71306
* Total *		0.00000	35.98237	91.71072	0.30691	128.00000

Natural Population	
Core	35.98237 ( 99.9510% of 36)
Valence	91.71072 ( 99.6856% of 92)
Natural Minimal Basis	127.69309 ( 99.7602% of 128)
Natural Rydberg Basis	0.30691 ( 0.2398% of 128)

Atom	No	Natural Electron Configuration
N	1	[core]2S( 1.20)2p( 4.06)3p( 0.01)
C	2	[core]2S( 0.94)2p( 2.83)4p( 0.01)
N	3	[core]2S( 1.20)2p( 4.05)3p( 0.01)
C	4	[core]2S( 0.96)2p( 3.12)3p( 0.01)
C	5	[core]2S( 0.96)2p( 3.12)3p( 0.01)
B	6	[core]2S( 0.63)2p( 2.57)
C	7	[core]2S( 0.90)2p( 2.95)3p( 0.02)4S( 0.01)3d( 0.01)
O	8	[core]2S( 1.70)2p( 4.88)3p( 0.01)



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C   9   [core]2S( 1.10)2p( 3.34)
C  10   [core]2S( 1.10)2p( 3.34)
B  11   [core]2S( 0.66)2p( 2.36)3p( 0.01)
C  12   [core]2S( 0.94)2p( 2.91)4p( 0.01)
N  13   [core]2S( 1.20)2p( 4.08)3p( 0.01)
C  14   [core]2S( 0.95)2p( 3.13)3p( 0.01)
C  15   [core]2S( 0.95)2p( 3.14)3p( 0.01)
N  16   [core]2S( 1.20)2p( 4.08)3p( 0.01)
C  17   [core]2S( 1.10)2p( 3.33)
C  18   [core]2S( 1.09)2p( 3.33)
H  19   1S( 0.77)
H  20   1S( 0.77)
H  21   1S( 0.77)
H  22   1S( 0.77)
H  23   1S( 0.79)
H  24   1S( 0.79)
H  25   1S( 0.73)
H  26   1S( 0.79)
H  27   1S( 0.79)
H  28   1S( 0.75)
H  29   1S( 0.79)
H  30   1S( 0.73)
H  31   1S( 0.79)
H  32   1S( 0.79)
H  33   1S( 0.79)
H  34   1S( 0.71)

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NATURAL BOND ORBITAL ANALYSIS:

Cycle	Occ. Thresh.	Occupancies		Lewis Structure				Low occ (L)	High occ (NL)	Dev
		Lewis	Non-Lewis	CR	BD	3C	LP			
1(1)	1.90	121.40551	6.59449	18	37	0	9	9	9	1.25
2(2)	1.90	121.40551	6.59449	18	37	0	9	9	9	1.25
3(1)	1.80	122.76499	5.23501	18	43	0	3	4	7	0.92
4(2)	1.80	122.76499	5.23501	18	43	0	3	4	7	0.92
5(1)	1.70	123.46656	4.53344	18	42	0	4	3	7	0.62
6(2)	1.70	123.92151	4.07849	18	41	0	5	3	7	0.25
7(3)	1.70	123.92151	4.07849	18	41	0	5	3	7	0.25
8(1)	1.60	122.19793	5.80207	18	43	0	3	4	10	0.25
9(2)	1.60	122.74581	5.25419	18	42	0	4	4	9	0.25
10(3)	1.60	122.74581	5.25419	18	42	0	4	4	9	0.25
11(1)	1.50	123.09997	4.90003	18	38	0	8	1	7	0.58
12(2)	1.50	123.09997	4.90003	18	38	0	8	1	7	0.58
13(1)	1.70	123.92151	4.07849	18	41	0	5	3	7	0.25

Structure accepted: RESONANCE keyword permits strongly delocalized structure

```

WARNING:  1 low occupancy (<1.9990e) core orbital found on C   2
          1 low occupancy (<1.9990e) core orbital found on B   6
          1 low occupancy (<1.9990e) core orbital found on C   7
          1 low occupancy (<1.9990e) core orbital found on B  11
          1 low occupancy (<1.9990e) core orbital found on C  12

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Core                35.98238 ( 99.951% of 36)
Valence Lewis      87.93913 ( 95.586% of 92)
=====
Total Lewis        123.92151 ( 96.814% of 128)
-----
Valence non-Lewis   3.86264 (  3.018% of 128)
Rydberg non-Lewis   0.21585 (  0.169% of 128)
=====
Total non-Lewis     4.07849 (  3.186% of 128)
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(Occupancy) Bond orbital/ Coefficients/ Hybrids

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-----
1. (1.98001) BD ( 1) N   1 - C   2
   ( 62.41%)  0.7900* N   1 s( 34.50%)p 1.90( 65.45%)d 0.00(  0.06%)
                                     -0.0001  0.5873  0.0058 -0.0055  0.0001
                                     -0.3369  0.0120  0.0004  0.6846  0.0052
                                     -0.0072 -0.2686 -0.0014  0.0024 -0.0102
                                     0.0042 -0.0135 -0.0133 -0.0098
   ( 37.59%)  0.6131* C   2 s( 26.95%)p 2.71( 72.97%)d 0.00(  0.07%)
                                     -0.0003  0.5185  0.0253  0.0003  0.0001
                                     0.2518 -0.0114 -0.0011 -0.7624 -0.0194
                                     -0.0172  0.2903  0.0065  0.0062 -0.0184
                                     0.0071 -0.0123 -0.0110 -0.0093

2. (1.98425) BD ( 1) N   1 - C   5
   ( 61.73%)  0.7857* N   1 s( 32.56%)p 2.07( 67.39%)d 0.00(  0.05%)
                                     0.0000  0.5706 -0.0027  0.0014  0.0000
                                     0.8154 -0.0015 -0.0034 -0.0606  0.0166
                                     -0.0099  0.0703 -0.0060  0.0033  0.0033
                                     0.0013  0.0000  0.0200 -0.0116
   ( 38.27%)  0.6187* C   5 s( 28.77%)p 2.47( 71.15%)d 0.00(  0.08%)
                                     -0.0001  0.5362  0.0119 -0.0034 -0.0010
                                     -0.8370 -0.0353  0.0069 -0.0916 -0.0221
                                     -0.0122 -0.0224  0.0056  0.0048 -0.0028
                                     0.0044 -0.0017  0.0233 -0.0155

3. (1.99022) BD ( 1) N   1 - C  10
   ( 62.61%)  0.7913* N   1 s( 32.89%)p 2.04( 67.08%)d 0.00(  0.02%)
                                     -0.0001  0.5735 -0.0077  0.0034 -0.0001
                                     -0.4666 -0.0020  0.0083 -0.6411  0.0001
                                     0.0020  0.2048 -0.0002 -0.0004  0.0126
                                     -0.0040 -0.0051 -0.0024 -0.0066
   ( 37.39%)  0.6115* C  10 s( 24.82%)p 3.03( 75.10%)d 0.00(  0.08%)
                                     0.0001  0.4975  0.0259 -0.0006 -0.0002
                                     0.5328  0.0212 -0.0041  0.6492  0.0194
                                     -0.0050 -0.2117 -0.0063  0.0016  0.0219
                                     -0.0072 -0.0091 -0.0050 -0.0114

4. (1.98001) BD ( 1) C   2 - N   3
   ( 37.65%)  0.6136* C   2 s( 26.62%)p 2.75( 73.30%)d 0.00(  0.07%)
                                     0.0003 -0.5154 -0.0240 -0.0016 -0.0001
                                     -0.6675 -0.0040 -0.0086 -0.5164 -0.0223
                                     -0.0138  0.1415  0.0075  0.0042 -0.0193
                                     0.0049  0.0025 -0.0130  0.0131
   ( 62.35%)  0.7896* N   3 s( 34.61%)p 1.89( 65.33%)d 0.00(  0.06%)
                                     0.0001 -0.5883 -0.0057  0.0047 -0.0001
                                     0.6902 -0.0070 -0.0039  0.4080  0.0117
                                     -0.0060 -0.1012 -0.0043  0.0020 -0.0187
                                     0.0047  0.0055 -0.0048  0.0127

5. (1.85099) BD ( 2) C   2 - N   3
   ( 26.76%)  0.5173* C   2 s(  0.00%)p 1.00( 99.85%)d 0.00(  0.15%)
                                     0.0000  0.0030  0.0004  0.0003  0.0000
                                     -0.0648 -0.0029  0.0008  0.3377  0.0114
                                     -0.0036  0.9375  0.0328 -0.0101  0.0118
                                     0.0347  0.0113 -0.0068 -0.0037
   ( 73.24%)  0.8558* N   3 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                                     0.0000  0.0017  0.0000 -0.0002  0.0000
                                     -0.0624  0.0000 -0.0005  0.3408 -0.0002
                                     0.0031  0.9379 -0.0006  0.0085 -0.0014
                                     -0.0063 -0.0102  0.0046  0.0065

6. (1.96108) BD ( 1) C   2 - B   6
   ( 65.58%)  0.8098* C   2 s( 46.47%)p 1.15( 53.53%)d 0.00(  0.00%)
                                     0.0000 -0.6815  0.0174  0.0024  0.0000
                                     0.6960 -0.0350 -0.0114 -0.1881  0.0105
                                     0.0033  0.1179 -0.0043 -0.0030  0.0024
                                     -0.0023  0.0016 -0.0038  0.0039
   ( 34.42%)  0.5866* B   6 s( 36.56%)p 1.73( 63.40%)d 0.00(  0.04%)
                                     0.0011 -0.6046 -0.0014  0.0031 -0.0022
                                     -0.7492 -0.0073 -0.0129  0.2380  0.0031
                                     0.0041 -0.1257 -0.0028 -0.0026  0.0083
                                     -0.0050  0.0020 -0.0145  0.0110

7. (1.98403) BD ( 1) N   3 - C   4
   ( 61.60%)  0.7848* N   3 s( 32.32%)p 2.09( 67.62%)d 0.00(  0.06%)
                                     0.0000  0.5685 -0.0034  0.0008  0.0000
                                     0.7202 -0.0118  0.0028 -0.3551 -0.0133

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					0.0101	0.1759	0.0041	-0.0034	-0.0181
					0.0080	-0.0060	0.0059	-0.0096	
	( 38.40%)	0.6197* C	4 s( 28.88%)	p 2.46( 71.03%)	d 0.00( 0.08%)				
					-0.0001	0.5373	0.0119	-0.0033	-0.0010
					-0.6505	-0.0162	0.0129	0.4883	0.0359
					0.0068	-0.2164	-0.0138	-0.0014	-0.0177
					0.0090	-0.0060	0.0137	-0.0140	
8.	(1.98983)	BD ( 1) N	3 - C	9					
	( 63.04%)	0.7940* N	3 s( 33.01%)	p 2.03( 66.97%)	d 0.00( 0.02%)				
					-0.0001	0.5745	-0.0066	0.0033	-0.0001
					-0.0059	-0.0007	0.0051	0.7686	0.0021
					-0.0056	-0.2807	-0.0008	0.0024	-0.0013
					0.0005	-0.0087	-0.0114	-0.0050	
	( 36.96%)	0.6079* C	9 s( 24.53%)	p 3.07( 75.40%)	d 0.00( 0.08%)				
					0.0001	0.4945	0.0269	-0.0013	-0.0002
					0.0376	0.0061	-0.0014	-0.8133	-0.0289
					0.0069	0.3002	0.0110	-0.0024	-0.0020
					0.0007	-0.0155	-0.0210	-0.0088	
9.	(1.97894)	BD ( 1) C	4 - C	5					
	( 49.96%)	0.7069* C	4 s( 37.00%)	p 1.70( 62.93%)	d 0.00( 0.06%)				
					0.0001	-0.6083	-0.0065	-0.0006	-0.0001
					0.1378	-0.0167	-0.0206	0.7380	0.0273
					-0.0041	-0.2532	-0.0109	0.0002	-0.0155
					0.0047	0.0112	0.0108	0.0114	
	( 50.04%)	0.7074* C	5 s( 37.07%)	p 1.70( 62.87%)	d 0.00( 0.06%)				
					0.0001	-0.6088	-0.0062	-0.0007	-0.0001
					-0.3192	-0.0301	-0.0151	-0.6882	-0.0153
					0.0137	0.2272	0.0034	-0.0058	-0.0052
					0.0015	0.0141	0.0173	0.0104	
10.	(1.87415)	BD ( 2) C	4 - C	5					
	( 49.80%)	0.7057* C	4 s( 0.00%)	p 1.00( 99.96%)	d 0.00( 0.04%)				
					0.0000	0.0005	0.0005	-0.0001	0.0000
					-0.0612	0.0022	-0.0011	0.3341	-0.0125
					0.0060	0.9394	-0.0352	0.0168	-0.0028
					-0.0109	-0.0128	0.0059	0.0078	
	( 50.20%)	0.7085* C	5 s( 0.00%)	p 1.00( 99.96%)	d 0.00( 0.04%)				
					0.0000	0.0011	0.0004	0.0000	0.0000
					-0.0613	0.0023	-0.0011	0.3372	-0.0127
					0.0060	0.9383	-0.0357	0.0169	-0.0013
					0.0000	0.0150	-0.0061	-0.0108	
11.	(1.98232)	BD ( 1) C	4 - H	19					
	( 61.69%)	0.7854* C	4 s( 34.06%)	p 1.94( 65.92%)	d 0.00( 0.02%)				
					-0.0003	0.5835	-0.0105	0.0013	0.0006
					0.7432	-0.0076	-0.0056	0.3198	-0.0086
					-0.0075	-0.0656	0.0026	0.0023	0.0102
					-0.0024	-0.0001	0.0078	-0.0058	
	( 38.31%)	0.6190* H	19 s( 99.94%)	p 0.00( 0.06%)					
					0.9997	0.0015	0.0002	-0.0229	-0.0095
					0.0019				
12.	(1.98252)	BD ( 1) C	5 - H	20					
	( 61.63%)	0.7851* C	5 s( 34.12%)	p 1.93( 65.86%)	d 0.00( 0.02%)				
					0.0003	-0.5840	0.0103	-0.0014	-0.0006
					-0.4361	0.0005	0.0005	0.6346	-0.0109
					-0.0091	-0.2559	0.0039	0.0033	0.0105
					-0.0040	0.0058	0.0055	0.0037	
	( 38.37%)	0.6194* H	20 s( 99.94%)	p 0.00( 0.06%)					
					-0.9997	-0.0017	-0.0006	0.0139	-0.0192
					0.0078				
13.	(1.89970)	BD ( 1) B	6 - C	7					
	( 40.18%)	0.6339* B	6 s( 28.33%)	p 2.53( 71.61%)	d 0.00( 0.06%)				
					-0.0009	0.5323	-0.0027	0.0037	-0.0007
					-0.1303	0.0092	-0.0041	0.7668	0.0056
					0.0098	-0.3330	-0.0004	-0.0053	-0.0139
					0.0060	-0.0092	-0.0087	-0.0141	
	( 59.82%)	0.7734* C	7 s( 39.27%)	p 1.55( 60.71%)	d 0.00( 0.02%)				
					-0.0002	0.6254	-0.0385	0.0021	-0.0004
					0.6986	0.0031	-0.0002	-0.3441	-0.0064
					0.0066	0.0222	-0.0012	-0.0024	-0.0125
					0.0040	-0.0029	-0.0026	-0.0065	
14.	(1.82653)	BD ( 1) B	6 - B	11					
	( 49.91%)	0.7065* B	6 s( 34.70%)	p 1.88( 65.28%)	d 0.00( 0.03%)				

					-0.0005	-0.5890	-0.0067	0.0007	0.0009
					0.6430	-0.0077	-0.0119	0.4816	-0.0043
					0.0048	-0.0839	-0.0015	-0.0012	0.0000
					0.0010	0.0022	-0.0143	0.0064	
	( 50.09%)	0.7077*	B	11	s( 40.21%)	p 1.49( 59.76%)	d 0.00( 0.02%)		
					-0.0001	-0.6341	0.0031	-0.0001	0.0006
					-0.6572	-0.0120	0.0145	0.4042	-0.0202
					0.0056	-0.0380	0.0075	-0.0049	-0.0067
					0.0049	-0.0006	-0.0112	0.0051	
15.	(1.99656)	BD ( 1)	C	7 - O	8				
	( 35.73%)	0.5978*	C	7	s( 33.83%)	p 1.95( 66.08%)	d 0.00( 0.09%)		
					-0.0003	0.5766	0.0766	0.0013	0.0010
					-0.1172	0.0090	-0.0016	0.7975	-0.0521
					0.0063	-0.0894	0.0159	0.0007	-0.0083
					0.0009	-0.0059	-0.0251	-0.0134	
	( 64.27%)	0.8017*	O	8	s( 38.87%)	p 1.57( 61.00%)	d 0.00( 0.13%)		
					0.0000	0.6232	-0.0183	0.0046	0.0001
					0.1123	-0.0038	-0.0007	-0.7057	0.0322
					-0.0020	0.3132	-0.0101	-0.0007	-0.0087
					0.0032	-0.0179	-0.0275	-0.0117	
16.	(1.98543)	BD ( 2)	C	7 - O	8				
	( 28.21%)	0.5311*	C	7	s( 0.61%)	p99.99( 99.15%)	d 0.39( 0.24%)		
					0.0002	-0.0764	-0.0157	0.0039	0.0002
					0.1280	-0.0021	-0.0009	0.1848	0.0124
					0.0030	0.9698	-0.0008	0.0184	0.0041
					-0.0102	0.0424	-0.0111	-0.0181	
	( 71.79%)	0.8473*	O	8	s( 0.47%)	p99.99( 99.43%)	d 0.21( 0.10%)		
					0.0000	-0.0682	0.0041	0.0001	-0.0001
					0.1246	-0.0031	-0.0006	0.3669	-0.0092
					0.0000	0.9187	-0.0127	-0.0021	-0.0016
					0.0051	-0.0243	0.0123	0.0149	
17.	(1.74346)	BD ( 1)	C	7 - B	11				
	( 59.19%)	0.7693*	C	7	s( 26.79%)	p 2.73( 73.18%)	d 0.00( 0.03%)		
					-0.0001	-0.5172	0.0213	0.0033	0.0001
					0.6932	0.0041	-0.0008	0.4508	0.0179
					-0.0065	-0.2180	-0.0102	0.0006	-0.0120
					0.0049	0.0065	0.0048	0.0070	
	( 40.81%)	0.6388*	B	11	s( 20.12%)	p 3.97( 79.83%)	d 0.00( 0.05%)		
					0.0038	-0.4483	0.0134	-0.0038	0.0044
					-0.0996	0.0058	0.0066	-0.8375	0.0007
					-0.0084	0.2944	-0.0018	0.0122	-0.0082
					0.0000	0.0101	0.0095	0.0166	
18.	(1.98423)	BD ( 1)	C	9 - H	32				
	( 60.68%)	0.7790*	C	9	s( 24.29%)	p 3.12( 75.67%)	d 0.00( 0.04%)		
					-0.0001	0.4928	-0.0065	0.0019	0.0002
					0.3921	-0.0096	0.0009	0.5272	0.0065
					0.0061	0.5699	-0.0066	0.0011	0.0090
					0.0117	0.0131	-0.0010	0.0053	
	( 39.32%)	0.6271*	H	32	s( 99.95%)	p 0.00( 0.05%)			
					0.9998	0.0020	0.0002	-0.0078	-0.0144
					-0.0142				
19.	(1.98400)	BD ( 1)	C	9 - H	33				
	( 60.69%)	0.7791*	C	9	s( 24.33%)	p 3.11( 75.63%)	d 0.00( 0.04%)		
					-0.0001	0.4932	-0.0065	0.0019	0.0001
					0.4265	-0.0101	0.0016	0.0395	0.0090
					0.0040	-0.7567	0.0001	-0.0045	-0.0005
					-0.0156	0.0016	0.0045	0.0124	
	( 39.31%)	0.6269*	H	33	s( 99.95%)	p 0.00( 0.05%)			
					0.9998	0.0022	0.0002	-0.0088	-0.0018
					0.0197				
20.	(1.98391)	BD ( 1)	C	9 - H	34				
	( 64.48%)	0.8030*	C	9	s( 26.91%)	p 2.71( 73.04%)	d 0.00( 0.04%)		
					0.0001	-0.5187	0.0035	0.0026	0.0001
					0.8137	-0.0120	-0.0068	-0.2375	-0.0028
					-0.0079	0.1082	0.0009	0.0024	0.0058
					-0.0029	-0.0007	-0.0176	0.0092	
	( 35.52%)	0.5960*	H	34	s( 99.94%)	p 0.00( 0.06%)			
					-0.9997	-0.0021	-0.0003	-0.0240	0.0049
					-0.0025				
21.	(1.98512)	BD ( 1)	C	10 - H	29				
	( 60.74%)	0.7794*	C	10	s( 24.52%)	p 3.08( 75.44%)	d 0.00( 0.04%)		

				-0.0001	0.4951	-0.0079	0.0020	0.0001
				0.1481	-0.0110	-0.0034	-0.2313	-0.0025
				-0.0033	0.8239	-0.0061	0.0053	-0.0017
				0.0078	-0.0069	0.0003	0.0176	
	( 39.26%)	0.6266*	H 29	s( 99.95%)	p 0.00( 0.05%)			
				0.9998	0.0023	0.0002	-0.0019	0.0051
				-0.0208				
22.	(1.98351)	BD ( 1)	C 10 - H 30					
	( 63.78%)	0.7987*	C 10	s( 26.23%)	p 2.81( 73.73%)	d 0.00( 0.04%)		
				0.0001	-0.5122	0.0007	0.0036	0.0000
				0.8167	-0.0038	-0.0028	-0.2486	0.0085
				0.0090	0.0910	-0.0035	-0.0032	0.0135
				-0.0046	0.0017	-0.0116	0.0090	
	( 36.22%)	0.6018*	H 30	s( 99.95%)	p 0.00( 0.05%)			
				-0.9997	-0.0018	-0.0009	-0.0197	0.0099
				-0.0035				
23.	(1.98503)	BD ( 1)	C 10 - H 31					
	( 60.68%)	0.7789*	C 10	s( 24.49%)	p 3.08( 75.47%)	d 0.00( 0.04%)		
				0.0001	-0.4948	0.0080	-0.0023	-0.0001
				-0.1611	0.0106	0.0028	0.6791	-0.0016
				0.0061	0.5170	-0.0059	0.0022	0.0066
				0.0053	-0.0165	0.0087	-0.0022	
	( 39.32%)	0.6271*	H 31	s( 99.95%)	p 0.00( 0.05%)			
				-0.9998	-0.0025	-0.0002	0.0026	-0.0166
				-0.0135				
24.	(1.96884)	BD ( 1)	B 11 - C 12					
	( 33.88%)	0.5820*	B 11	s( 39.46%)	p 1.53( 60.49%)	d 0.00( 0.05%)		
				-0.0003	0.6281	0.0102	0.0017	0.0042
				-0.7398	-0.0165	-0.0138	-0.2056	-0.0036
				-0.0051	0.1214	0.0024	0.0037	0.0073
				-0.0053	-0.0003	0.0182	-0.0114	
	( 66.12%)	0.8132*	C 12	s( 46.47%)	p 1.15( 53.52%)	d 0.00( 0.01%)		
				-0.0001	0.6815	-0.0161	-0.0066	0.0000
				0.7231	-0.0379	-0.0074	0.0878	-0.0059
				-0.0017	-0.0551	0.0012	0.0018	0.0033
				-0.0028	0.0032	0.0061	-0.0035	
25.	(1.97811)	BD ( 1)	C 12 - N 13					
	( 38.05%)	0.6169*	C 12	s( 26.73%)	p 2.74( 73.20%)	d 0.00( 0.07%)		
				-0.0003	0.5165	0.0208	0.0058	0.0000
				-0.5084	-0.0003	-0.0015	0.4869	0.0186
				0.0113	0.4854	0.0159	0.0101	-0.0160
				-0.0159	0.0125	0.0070	-0.0045	
	( 61.95%)	0.7871*	N 13	s( 33.66%)	p 1.97( 66.28%)	d 0.00( 0.06%)		
				-0.0001	0.5801	0.0063	-0.0066	0.0001
				0.5611	-0.0101	-0.0040	-0.4027	-0.0046
				0.0071	-0.4308	-0.0053	0.0061	-0.0129
				-0.0132	0.0154	0.0019	-0.0019	
26.	(1.84802)	BD ( 2)	C 12 - N 13					
	( 25.65%)	0.5065*	C 12	s( 0.00%)	p 1.00( 99.85%)	d 0.00( 0.15%)		
				0.0002	0.0054	0.0016	-0.0014	0.0002
				0.1298	0.0100	-0.0060	-0.6309	-0.0207
				0.0037	0.7632	0.0244	-0.0060	0.0221
				-0.0215	0.0008	0.0040	0.0222	
	( 74.35%)	0.8622*	N 13	s( 0.00%)	p 1.00( 99.98%)	d 0.00( 0.02%)		
				0.0000	0.0002	0.0003	-0.0006	0.0000
				0.1266	0.0000	0.0013	-0.6367	-0.0008
				-0.0058	0.7605	0.0015	0.0076	-0.0031
				0.0008	-0.0024	-0.0054	-0.0111	
27.	(1.97905)	BD ( 1)	C 12 - N 16					
	( 37.97%)	0.6162*	C 12	s( 26.81%)	p 2.73( 73.12%)	d 0.00( 0.07%)		
				-0.0003	0.5173	0.0219	0.0066	0.0000
				-0.4467	0.0046	0.0000	-0.5953	-0.0188
				-0.0125	-0.4200	-0.0148	-0.0098	0.0190
				0.0123	0.0133	0.0021	-0.0057	
	( 62.03%)	0.7876*	N 16	s( 34.05%)	p 1.93( 65.89%)	d 0.00( 0.06%)		
				-0.0001	0.5835	0.0069	-0.0062	0.0001
				0.5204	-0.0104	-0.0035	0.4826	0.0041
				-0.0078	0.3936	0.0047	-0.0059	0.0147
				0.0090	0.0157	-0.0021	-0.0041	
28.	(1.98342)	BD ( 1)	N 13 - C 14					
	( 61.68%)	0.7854*	N 13	s( 33.09%)	p 2.02( 66.86%)	d 0.00( 0.05%)		

					0.0000	0.5752	-0.0018	0.0024	0.0000
					-0.7870	0.0084	-0.0006	-0.2153	-0.0120
					0.0088	-0.0494	-0.0103	0.0075	0.0135
					0.0060	0.0029	0.0138	-0.0108	
	( 38.32%)	0.6190*	C 14	s( 28.77%)p 2.47( 71.16%)d 0.00( 0.08%)	-0.0001	0.5362	0.0110	-0.0027	-0.0012
					0.7622	0.0259	-0.0105	0.3142	0.0267
					0.0075	0.1729	0.0196	0.0076	0.0113
					0.0037	0.0033	0.0211	-0.0138	
29.	(1.99041)	BD ( 1)	N 13 - C 17						
	( 62.43%)	0.7901*	N 13	s( 33.19%)p 2.01( 66.78%)d 0.00( 0.03%)	-0.0001	0.5761	-0.0086	0.0034	-0.0001
					0.2210	0.0029	-0.0073	0.6210	-0.0012
					-0.0036	0.4830	-0.0016	-0.0017	0.0068
					0.0053	0.0124	-0.0057	-0.0002	
	( 37.57%)	0.6130*	C 17	s( 25.24%)p 2.96( 74.68%)d 0.00( 0.08%)	0.0001	0.5017	0.0265	-0.0018	-0.0002
					-0.2565	-0.0124	0.0008	-0.6701	-0.0221
					0.0059	-0.4807	-0.0142	0.0034	0.0108
					0.0081	0.0206	-0.0124	-0.0013	
30.	(1.97858)	BD ( 1)	C 14 - C 15						
	( 50.01%)	0.7072*	C 14	s( 37.28%)p 1.68( 62.65%)d 0.00( 0.06%)	0.0001	-0.6106	-0.0066	-0.0007	-0.0002
					0.0647	0.0234	0.0183	0.5996	0.0203
					-0.0056	0.5111	0.0148	-0.0073	0.0052
					0.0055	-0.0222	0.0090	-0.0028	
	( 49.99%)	0.7070*	C 15	s( 37.32%)p 1.68( 62.62%)d 0.00( 0.06%)	0.0001	-0.6109	-0.0068	-0.0009	-0.0002
					0.1179	0.0243	0.0185	-0.5701	-0.0177
					0.0084	-0.5344	-0.0181	0.0052	-0.0040
					-0.0031	-0.0225	0.0099	-0.0024	
31.	(1.90232)	BD ( 2)	C 14 - C 15						
	( 49.43%)	0.7031*	C 14	s( 0.00%)p 1.00( 99.96%)d 0.00( 0.04%)	0.0001	-0.0061	-0.0024	0.0005	0.0000
					0.1047	-0.0040	0.0018	-0.6546	0.0253
					-0.0113	0.7473	-0.0275	0.0128	-0.0048
					0.0029	-0.0017	-0.0081	-0.0168	
	( 50.57%)	0.7111*	C 15	s( 0.00%)p 1.00( 99.96%)d 0.00( 0.04%)	-0.0001	-0.0047	0.0000	0.0000	0.0000
					0.0960	-0.0030	0.0017	-0.6666	0.0266
					-0.0116	0.7377	-0.0293	0.0116	-0.0013
					0.0045	0.0021	0.0099	0.0155	
32.	(1.98166)	BD ( 1)	C 14 - H 21						
	( 61.46%)	0.7839*	C 14	s( 33.90%)p 1.95( 66.08%)d 0.00( 0.02%)	0.0003	-0.5821	0.0101	-0.0007	-0.0007
					0.6336	-0.0044	-0.0036	-0.3330	0.0072
					0.0063	-0.3851	0.0075	0.0057	0.0092
					0.0098	-0.0040	-0.0042	0.0012	
	( 38.54%)	0.6208*	H 21	s( 99.94%)p 0.00( 0.06%)	-0.9997	-0.0016	-0.0003	-0.0200	0.0097
					0.0116				
33.	(1.98310)	BD ( 1)	C 15 - N 16						
	( 38.27%)	0.6186*	C 15	s( 28.57%)p 2.50( 71.35%)d 0.00( 0.08%)	-0.0001	0.5344	0.0113	-0.0031	-0.0011
					0.7864	0.0298	-0.0094	-0.1705	-0.0216
					-0.0099	-0.2529	-0.0214	-0.0066	-0.0029
					-0.0086	0.0030	0.0232	-0.0129	
	( 61.73%)	0.7857*	N 16	s( 32.78%)p 2.05( 67.17%)d 0.00( 0.05%)	0.0000	0.5725	-0.0007	0.0023	0.0000
					-0.8040	0.0076	0.0005	0.0538	0.0115
					-0.0085	0.1484	0.0097	-0.0079	-0.0073
					-0.0094	0.0027	0.0170	-0.0094	
34.	(1.98163)	BD ( 1)	C 15 - H 22						
	( 61.44%)	0.7838*	C 15	s( 34.05%)p 1.94( 65.93%)d 0.00( 0.02%)	-0.0003	0.5835	-0.0104	0.0008	0.0006
					-0.5964	0.0022	0.0033	-0.4467	0.0077
					0.0070	-0.3223	0.0059	0.0064	0.0106
					0.0079	0.0048	0.0017	-0.0030	
	( 38.56%)	0.6210*	H 22	s( 99.94%)p 0.00( 0.06%)	0.9997	0.0016	0.0002	0.0189	0.0130
					0.0100				

35. (1.99096) BD ( 1) N 16 - C 18  
( 62.04%) 0.7877\* N 16 s( 33.11%)p 2.02( 66.86%)d 0.00( 0.03%)  
-0.0001 0.5754 -0.0098 0.0031 -0.0001  
0.2725 0.0013 -0.0074 -0.5435 0.0018  
0.0018 -0.5466 0.0023 0.0035 -0.0061  
-0.0076 0.0127 -0.0027 0.0040  
( 37.96%) 0.6161\* C 18 s( 25.65%)p 2.90( 74.28%)d 0.00( 0.08%)  
0.0001 0.5058 0.0261 0.0000 -0.0002  
-0.3175 -0.0135 0.0015 0.5550 0.0159  
-0.0039 0.5772 0.0192 -0.0026 -0.0107  
-0.0114 0.0210 -0.0066 0.0052

36. (1.98684) BD ( 1) C 17 - H 23  
( 60.57%) 0.7783\* C 17 s( 24.24%)p 3.12( 75.72%)d 0.00( 0.04%)  
-0.0001 0.4923 -0.0047 0.0026 0.0003  
-0.6870 0.0103 0.0034 0.5038 0.0053  
0.0053 0.1769 0.0015 0.0028 -0.0148  
-0.0041 0.0029 0.0085 -0.0095  
( 39.43%) 0.6279\* H 23 s( 99.95%)p 0.00( 0.05%)  
0.9997 0.0013 0.0002 0.0166 -0.0150  
-0.0043

37. (1.98534) BD ( 1) C 17 - H 24  
( 60.75%) 0.7794\* C 17 s( 24.62%)p 3.06( 75.34%)d 0.00( 0.04%)  
-0.0001 0.4962 -0.0058 0.0008 -0.0001  
0.3335 0.0059 -0.0038 -0.2921 0.0094  
0.0018 0.7460 -0.0047 0.0078 -0.0070  
0.0104 -0.0114 0.0003 0.0117  
( 39.25%) 0.6265\* H 24 s( 99.96%)p 0.00( 0.04%)  
0.9998 0.0043 0.0002 -0.0090 0.0071  
-0.0175

38. (1.98070) BD ( 1) C 17 - H 25  
( 63.33%) 0.7958\* C 17 s( 25.95%)p 2.85( 74.01%)d 0.00( 0.05%)  
-0.0001 0.5093 -0.0061 -0.0020 -0.0001  
0.5918 -0.0041 -0.0068 0.4582 -0.0033  
0.0104 -0.4238 0.0109 0.0024 0.0098  
-0.0149 -0.0107 0.0043 -0.0020  
( 36.67%) 0.6056\* H 25 s( 99.94%)p 0.00( 0.06%)  
0.9997 0.0030 0.0000 -0.0167 -0.0106  
0.0136

39. (1.98702) BD ( 1) C 18 - H 26  
( 60.55%) 0.7782\* C 18 s( 24.44%)p 3.09( 75.52%)d 0.00( 0.04%)  
0.0001 -0.4943 0.0072 -0.0030 -0.0003  
0.4176 -0.0090 -0.0040 0.7589 -0.0017  
0.0054 -0.0680 0.0063 0.0016 -0.0152  
0.0026 0.0045 0.0072 0.0100  
( 39.45%) 0.6281\* H 26 s( 99.95%)p 0.00( 0.05%)  
-0.9997 -0.0023 -0.0003 -0.0094 -0.0201  
0.0019

40. (1.98581) BD ( 1) C 18 - H 27  
( 60.96%) 0.7808\* C 18 s( 24.84%)p 3.02( 75.12%)d 0.00( 0.04%)  
0.0001 -0.4983 0.0079 -0.0012 0.0002  
0.1120 -0.0097 0.0015 -0.3145 0.0080  
0.0013 0.7997 -0.0051 0.0072 0.0010  
-0.0047 0.0132 0.0022 -0.0147  
( 39.04%) 0.6248\* H 27 s( 99.96%)p 0.00( 0.04%)  
-0.9998 -0.0041 -0.0003 -0.0016 0.0085  
-0.0188

41. (1.98196) BD ( 1) C 18 - H 28  
( 62.37%) 0.7898\* C 18 s( 25.14%)p 2.98( 74.82%)d 0.00( 0.04%)  
-0.0001 0.5013 -0.0018 -0.0040 0.0000  
0.8434 -0.0038 -0.0055 -0.1246 -0.0002  
-0.0091 0.1451 -0.0099 -0.0029 -0.0016  
0.0090 -0.0014 0.0159 -0.0098  
( 37.63%) 0.6134\* H 28 s( 99.95%)p 0.00( 0.05%)  
0.9998 0.0029 0.0002 -0.0216 0.0005  
-0.0041

42. (1.99944) CR ( 1) N 1  
s(100.00%)  
1.0000 0.0001 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

43. (1.99879) CR ( 1) C 2  
s(100.00%)p 0.00( 0.00%)

				1.0000	0.0003	0.0000	0.0000	0.0000	0.0000
				0.0003	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
44.	(1.99944)	CR ( 1) N	3	s(100.00%)					
				1.0000	0.0001	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
				0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
45.	(1.99912)	CR ( 1) C	4	s(100.00%)p 0.00( 0.00%)					
				1.0000	0.0003	0.0000	0.0000	0.0000	0.0000
				0.0001	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
46.	(1.99911)	CR ( 1) C	5	s(100.00%)p 0.00( 0.00%)					
				1.0000	0.0003	0.0000	0.0000	0.0000	0.0000
				0.0001	0.0000	0.0000	-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
47.	(1.99710)	CR ( 1) B	6	s(100.00%)p 0.00( 0.00%)					
				1.0000	0.0009	0.0000	0.0000	0.0000	0.0000
				0.0011	0.0000	0.0000	0.0007	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
48.	(1.99861)	CR ( 1) C	7	s(100.00%)p 0.00( 0.00%)					
				1.0000	0.0002	0.0000	0.0000	0.0000	0.0000
				0.0001	0.0000	0.0000	0.0002	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
49.	(1.99982)	CR ( 1) O	8	s(100.00%)p 0.00( 0.00%)					
				1.0000	0.0003	0.0000	0.0000	0.0000	0.0000
				-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
50.	(1.99931)	CR ( 1) C	9	s(100.00%)p 0.00( 0.00%)					
				1.0000	0.0001	0.0000	0.0000	0.0000	0.0000
				0.0001	0.0000	0.0000	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
51.	(1.99933)	CR ( 1) C	10	s(100.00%)p 0.00( 0.00%)					
				1.0000	0.0001	0.0000	0.0000	0.0000	0.0000
				-0.0001	0.0000	0.0000	-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
52.	(1.99777)	CR ( 1) B	11	s(100.00%)p 0.00( 0.00%)					
				1.0000	0.0018	0.0000	0.0000	0.0000	0.0000
				0.0001	0.0000	0.0000	0.0032	0.0000	0.0000
				0.0000	-0.0011	0.0000	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	-0.0001	0.0000	0.0000
53.	(1.99873)	CR ( 1) C	12	s(100.00%)p 0.00( 0.00%)					
				1.0000	0.0004	0.0000	0.0000	0.0000	0.0000
				-0.0002	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
54.	(1.99946)	CR ( 1) N	13	s(100.00%)					
				1.0000	0.0001	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	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
55.	(1.99911)	CR ( 1) C	14	s(100.00%)p 0.00( 0.00%)					
				1.0000	0.0003	0.0000	0.0000	0.0000	0.0000
				-0.0001	0.0000	0.0000	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
56.	(1.99911)	CR ( 1) C	15	s(100.00%)p 0.00( 0.00%)					
				1.0000	0.0003	0.0000	0.0000	0.0000	0.0000
				-0.0001	0.0000	0.0000	-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
57.	(1.99946)	CR ( 1) N	16	s(100.00%)					
				1.0000	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	0.0000	0.0000	0.0000
				0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
58.	(1.99933)	CR ( 1)	C 17	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	0.0001	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
59.	(1.99934)	CR ( 1)	C 18	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	-0.0001	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
60.	(1.52100)	LP ( 1)	N 1	s( 0.00%)	p 1.00( 99.99%)	d 0.00( 0.01%)			
				0.0000	-0.0002	-0.0002	0.0002	0.0000	0.0000
				0.0558	0.0004	0.0005	-0.3406	-0.0019	0.0000
				-0.0037	-0.9384	-0.0049	-0.0106	-0.0012	0.0000
				-0.0044	-0.0067	0.0030	0.0042	0.0000	0.0000
61.	(0.74739)	LP ( 1)	B 6	s( 0.31%)	p99.99( 99.62%)	d 0.21( 0.06%)			
				0.0000	0.0557	0.0034	-0.0013	-0.0004	0.0000
				-0.0897	0.0043	-0.0022	0.3500	-0.0006	0.0000
				0.0007	0.9303	0.0055	-0.0098	-0.0090	0.0000
				-0.0174	0.0150	-0.0025	-0.0049	0.0000	0.0000
62.	(1.96911)	LP ( 1)	O 8	s( 60.22%)	p 0.66( 39.76%)	d 0.00( 0.02%)			
				-0.0004	0.7760	0.0091	-0.0022	-0.0001	0.0000
				-0.1588	-0.0019	-0.0003	0.5898	0.0051	0.0000
				0.0054	-0.1565	-0.0003	-0.0011	0.0048	0.0000
				-0.0012	0.0061	0.0093	0.0064	0.0000	0.0000
63.	(1.77279)	LP ( 2)	O 8	s( 0.40%)	p99.99( 99.54%)	d 0.16( 0.06%)			
				0.0000	0.0633	0.0002	-0.0003	0.0000	0.0000
				0.9724	0.0174	-0.0027	0.1310	0.0025	0.0000
				0.0017	-0.1795	-0.0037	-0.0003	-0.0228	0.0000
				0.0060	0.0052	0.0069	-0.0027	0.0000	0.0000
64.	(0.61730)	LP*( 1)	B 11	s( 0.11%)	p99.99( 99.77%)	d 1.00( 0.11%)			
				0.0000	0.0334	-0.0013	0.0036	-0.0008	0.0000
				0.0993	0.0094	-0.0009	0.3028	-0.0058	0.0000
				-0.0039	0.9466	0.0008	-0.0091	0.0131	0.0000
				0.0174	0.0204	-0.0072	-0.0137	0.0000	0.0000
65.	(1.55922)	LP ( 1)	N 16	s( 0.00%)	p 1.00( 99.99%)	d 0.00( 0.01%)			
				0.0000	-0.0004	0.0012	-0.0004	-0.0001	0.0000
				0.0876	0.0000	0.0005	-0.6843	-0.0068	0.0000
				-0.0078	0.7237	0.0068	0.0095	0.0017	0.0000
				-0.0017	0.0012	0.0045	0.0065	0.0000	0.0000
66.	(0.00407)	RY*( 1)	N 1	s( 15.45%)	p 4.68( 72.34%)	d 0.79( 12.21%)			
				0.0000	-0.0104	0.3926	-0.0164	0.0002	0.0000
				-0.0101	0.3152	0.0293	-0.0137	0.7599	0.0000
				-0.0497	0.0040	-0.2063	0.0215	-0.3193	0.0000
				0.1198	0.0178	0.0714	0.0191	0.0000	0.0000
67.	(0.00243)	RY*( 2)	N 1	s( 0.05%)	p99.99( 98.06%)	d37.90( 1.89%)			
				0.0000	0.0008	0.0223	0.0018	-0.0001	0.0000
				0.0010	-0.1345	-0.0060	-0.0015	0.3145	0.0000
				0.0220	-0.0068	0.9274	0.0545	0.0664	0.0000
				0.0951	0.0361	-0.0623	-0.0167	0.0000	0.0000
68.	(0.00202)	RY*( 3)	N 1	s( 1.26%)	p62.86( 79.15%)	d15.56( 19.60%)			
				0.0000	0.0014	0.1058	0.0372	-0.0005	0.0000
				0.0027	-0.8107	-0.0532	0.0024	0.2721	0.0000
				0.0590	-0.0002	-0.2296	-0.0343	-0.0021	0.0000
				-0.0366	-0.1339	-0.4143	0.0711	0.0000	0.0000
69.	(0.00084)	RY*( 4)	N 1	s( 81.71%)	p 0.20( 16.63%)	d 0.02( 1.65%)			
				0.0000	0.0094	0.8917	0.1481	-0.0036	0.0000
				0.0061	-0.0122	-0.0175	-0.0052	-0.3923	0.0000
				-0.0248	0.0023	0.1052	-0.0148	0.0564	0.0000
				-0.0373	0.0684	-0.0596	0.0612	0.0000	0.0000
70.	(0.00063)	RY*( 5)	N 1	s( 0.10%)	p71.93( 7.04%)	d99.99( 92.86%)			
				0.0000	0.0003	0.0312	0.0016	0.0001	0.0000
				0.0005	0.0129	-0.0091	0.0007	-0.0212	0.0000
				0.0963	0.0025	-0.0103	0.2456	0.1958	0.0000
				0.3733	-0.6497	0.2350	0.5230	0.0000	0.0000
71.	(0.00040)	RY*( 6)	N 1	s( 0.03%)	p99.99( 4.16%)	d99.99( 95.81%)			
				0.0000	-0.0001	0.0162	0.0024	0.0001	0.0000
				-0.0002	-0.0051	-0.0150	0.0020	0.0373	0.0000

					0.0555	0.0045	0.1092	0.1579	-0.2575
					-0.8551	-0.3328	0.1817	0.1299	
72.	(0.00019)	RY*( 7)	N	1	s( 15.97%)	p 0.65( 10.40%)	d 4.61( 73.63%)		
					0.0000	-0.0065	0.0410	0.3971	0.0174
					-0.0142	-0.0829	0.0660	0.0185	0.2792
					0.0063	-0.0077	-0.1191	0.0018	0.7089
					-0.2039	0.1477	0.3981	-0.1088	
73.	(0.00015)	RY*( 8)	N	1	s( 2.64%)	p 8.69( 22.96%)	d28.17( 74.40%)		
					0.0000	-0.0048	-0.0383	0.1569	0.0171
					0.0189	0.4619	-0.0340	-0.0047	0.0845
					0.0727	0.0030	-0.0074	-0.0466	0.3501
					-0.1637	-0.2589	-0.7263	-0.0078	
74.	(0.00013)	RY*( 9)	N	1	s( 12.10%)	p 7.11( 86.05%)	d 0.15( 1.85%)		
					0.0000	0.0023	-0.0734	0.3395	-0.0186
					-0.0089	0.0253	-0.9084	-0.0041	0.0019
					-0.1856	0.0013	0.0084	0.0029	-0.1072
					0.0420	0.0309	0.0440	0.0487	
75.	(0.00006)	RY*(10)	N	1	s( 64.62%)	p 0.28( 17.86%)	d 0.27( 17.52%)		
76.	(0.00003)	RY*(11)	N	1	s( 4.03%)	p23.40( 94.31%)	d 0.41( 1.66%)		
77.	(0.00002)	RY*(12)	N	1	s( 3.43%)	p 0.22( 0.76%)	d27.90( 95.81%)		
78.	(0.00000)	RY*(13)	N	1	s( 0.12%)	p99.99( 90.14%)	d79.04( 9.74%)		
79.	(0.00000)	RY*(14)	N	1	s( 98.54%)	p 0.00( 0.25%)	d 0.01( 1.22%)		
80.	(0.00504)	RY*( 1)	C	2	s( 3.19%)	p28.30( 90.19%)	d 2.08( 6.63%)		
					0.0000	0.0172	0.1700	0.0516	-0.0016
					-0.0331	-0.8702	0.0402	0.0144	0.2040
					-0.0501	0.0010	-0.3004	0.0851	0.0812
					-0.1136	-0.0634	-0.2043	0.0322	
81.	(0.00255)	RY*( 2)	C	2	s( 10.76%)	p 5.59( 60.11%)	d 2.71( 29.13%)		
					0.0000	-0.0072	0.3261	-0.0347	-0.0009
					-0.0074	0.2496	-0.1771	0.0188	-0.2231
					0.0203	0.0428	-0.6491	0.1835	-0.2610
					-0.4200	-0.1339	0.1530	0.0738	
82.	(0.00211)	RY*( 3)	C	2	s( 38.54%)	p 1.07( 41.37%)	d 0.52( 20.09%)		
					0.0000	-0.0052	0.6133	-0.0960	0.0000
					-0.0159	0.0947	-0.4306	0.0112	0.3002
					-0.3100	-0.0273	0.1772	0.0232	-0.2226
					0.3457	0.0548	-0.1682	0.0242	
83.	(0.00192)	RY*( 4)	C	2	s( 10.94%)	p 8.04( 87.97%)	d 0.10( 1.09%)		
					0.0000	-0.0020	0.3251	-0.0609	-0.0016
					-0.0033	-0.2734	-0.1318	0.0247	-0.8173
					0.1345	-0.0138	0.3119	-0.0587	0.0626
					0.0447	0.0519	0.0474	-0.0025	
84.	(0.00113)	RY*( 5)	C	2	s( 11.81%)	p 3.40( 40.12%)	d 4.07( 48.07%)		
					0.0000	-0.0026	0.3417	0.0360	-0.0043
					-0.0212	0.0847	0.0816	-0.0308	0.1824
					0.5452	0.0012	-0.1952	-0.1319	0.2846
					0.0782	0.5522	0.0837	-0.2858	
85.	(0.00107)	RY*( 6)	C	2	s( 7.53%)	p 3.84( 28.97%)	d 8.43( 63.50%)		
					0.0000	-0.0001	0.2720	-0.0365	-0.0047
					-0.0179	-0.0088	0.0215	-0.0178	0.2663
					0.3514	0.0051	0.2226	-0.2111	0.2014
					-0.1090	-0.5085	0.3891	0.4154	
86.	(0.00042)	RY*( 7)	C	2	s( 3.53%)	p 8.72( 30.77%)	d18.63( 65.71%)		
					0.0000	0.0009	-0.0960	0.1614	-0.0023
					0.0052	0.0269	-0.0763	-0.0041	-0.1339
					0.0739	-0.0057	-0.3364	0.4056	0.2786
					0.6961	-0.1380	0.1454	0.2339	
87.	(0.00022)	RY*( 8)	C	2	s( 53.46%)	p 0.31( 16.70%)	d 0.56( 29.84%)		
					0.0000	-0.0017	0.1256	0.7202	-0.0074
					-0.0052	-0.0478	0.0578	-0.0014	0.0370
					-0.3324	0.0000	0.1695	0.1440	0.0207
					-0.1659	0.2381	0.4618	0.0216	
88.	(0.00017)	RY*( 9)	C	2	s( 16.11%)	p 2.42( 38.90%)	d 2.79( 45.00%)		
					0.0000	-0.0195	0.3632	0.1624	0.0485
					-0.0062	0.2649	0.5069	0.0014	-0.0777
					-0.1569	-0.0022	0.0489	0.1696	0.3711
					-0.0850	-0.2796	-0.4628	-0.1124	
89.	(0.00012)	RY*(10)	C	2	s( 7.97%)	p 3.80( 30.28%)	d 7.75( 61.75%)		
					0.0000	-0.0065	0.1021	0.2630	0.0092
					0.0012	-0.0578	0.4470	0.0135	-0.0257
					0.3044	-0.0056	-0.0014	-0.0783	-0.7188

					0.2913	-0.1117	-0.0589	-0.0040
90.	(0.00007)	R <sub>Y</sub> * (11)	C	2	s ( 31.01%)	p 1.05 ( 32.66%)	d 1.17 ( 36.33%)	
91.	(0.00005)	R <sub>Y</sub> * (12)	C	2	s ( 1.31%)	p70.34 ( 91.97%)	d 5.14 ( 6.72%)	
92.	(0.00002)	R <sub>Y</sub> * (13)	C	2	s ( 7.67%)	p 1.34 ( 10.31%)	d10.70 ( 82.03%)	
93.	(0.00000)	R <sub>Y</sub> * (14)	C	2	s ( 96.14%)	p 0.00 ( 0.05%)	d 0.04 ( 3.81%)	
94.	(0.00403)	R <sub>Y</sub> * ( 1)	N	3	s ( 12.46%)	p 6.02 ( 75.01%)	d 1.00 ( 12.52%)	
					0.0000	-0.0106	0.3528	-0.0056
					0.0003	-0.1548	0.0438	0.0172
					0.0212	-0.0063	0.2992	-0.0034
					0.0597	-0.0021	0.1226	-0.0191
95.	(0.00236)	R <sub>Y</sub> * ( 2)	N	3	s ( 0.05%)	p99.99 ( 97.81%)	d40.19 ( 2.14%)	
					0.0000	0.0006	0.0224	-0.0056
					-0.0003	-0.1936	-0.0189	-0.0010
					0.0271	-0.0003	0.8931	0.0607
					0.0846	0.0645	-0.0726	-0.0104
96.	(0.00199)	R <sub>Y</sub> * ( 3)	N	3	s ( 0.05%)	p99.99 ( 82.25%)	d99.99 ( 17.70%)	
					0.0000	0.0000	-0.0032	0.0222
					0.0006	0.8713	0.0856	0.0018
					0.0141	-0.0008	0.2323	0.0097
					-0.3584	0.1553	-0.0011	0.1561
97.	(0.00079)	R <sub>Y</sub> * ( 4)	N	3	s ( 83.40%)	p 0.15 ( 12.74%)	d 0.05 ( 3.86%)	
					0.0000	0.0091	0.9055	0.1185
					0.0101	0.1094	0.0256	-0.0007
					0.3093	-0.0295	-0.0001	-0.1296
					-0.0373	0.0642	-0.1352	-0.0107
98.	(0.00069)	R <sub>Y</sub> * ( 5)	N	3	s ( 1.17%)	p 6.48 ( 7.59%)	d77.94 ( 91.24%)	
					0.0000	0.0010	0.1072	0.0149
					-0.0007	0.0211	-0.0198	0.0035
					0.0183	0.1028	0.0089	-0.0550
					0.2471	0.2475	0.7513	0.4379
99.	(0.00041)	R <sub>Y</sub> * ( 6)	N	3	s ( 0.01%)	p 1.00 ( 3.78%)	d25.48 ( 96.22%)	
					0.0000	-0.0001	0.0077	-0.0053
					-0.0008	-0.0005	-0.0001	-0.0221
					0.0023	0.0430	0.0767	0.0049
					0.1138	0.1287	-0.2410	-0.5130
100.	(0.00020)	R <sub>Y</sub> * ( 7)	N	3	s ( 4.23%)	p 4.94 ( 20.90%)	d17.70 ( 74.87%)	
					0.0000	-0.0043	0.1049	0.1766
					0.0101	-0.0273	-0.3638	0.2567
					-0.0052	-0.0376	-0.0784	0.0002
					-0.0188	0.0454	-0.7881	0.2729
101.	(0.00014)	R <sub>Y</sub> * ( 8)	N	3	s ( 21.66%)	p 3.03 ( 65.56%)	d 0.59 ( 12.77%)	
					0.0000	0.0036	-0.0282	0.4640
					-0.0234	-0.0106	-0.0803	-0.5607
					0.0069	0.0837	0.5295	-0.0037
					-0.1730	0.0699	0.1088	0.2780
102.	(0.00015)	R <sub>Y</sub> * ( 9)	N	3	s ( 37.81%)	p 0.35 ( 13.37%)	d 1.29 ( 48.82%)	
					0.0000	-0.0058	-0.0521	0.6122
					0.0236	0.0060	0.1582	-0.0666
					-0.0079	-0.2903	-0.0680	0.0035
					0.1223	0.0168	0.2047	-0.1086
					-0.0086	0.3367%	p 1.14 ( 38.37%)	d 0.83 ( 27.96%)
103.	(0.00008)	R <sub>Y</sub> * (10)	N	3	s ( 4.79%)	p19.03 ( 91.17%)	d 0.84 ( 4.04%)	
104.	(0.00003)	R <sub>Y</sub> * (11)	N	3	s ( 2.18%)	p 0.38 ( 0.83%)	d44.46 ( 96.99%)	
105.	(0.00002)	R <sub>Y</sub> * (12)	N	3	s ( 0.02%)	p99.99 ( 90.52%)	d99.99 ( 9.46%)	
106.	(0.00000)	R <sub>Y</sub> * (13)	N	3	s ( 98.54%)	p 0.00 ( 0.20%)	d 0.01 ( 1.26%)	
107.	(0.00000)	R <sub>Y</sub> * (14)	N	3	s ( 0.02%)	p99.99 ( 82.54%)	d99.99 ( 17.43%)	
108.	(0.00384)	R <sub>Y</sub> * ( 1)	C	4	0.0000	0.0001	0.0146	0.0004
					0.0005	0.0023	0.0454	-0.0165
					-0.2982	0.0639	-0.0342	-0.8356
					0.1749	0.1316	0.3191	-0.1632
109.	(0.00300)	R <sub>Y</sub> * ( 2)	C	4	s ( 5.65%)	p14.91 ( 84.18%)	d 1.80 ( 10.18%)	
					0.0000	-0.0042	0.2369	0.0168
					0.0059	-0.0209	-0.5686	-0.0926
					0.0113	-0.6553	-0.1840	-0.0052
					0.2065	0.0587	0.1870	-0.0568
					0.0167	0.1424%	p 5.56 ( 79.24%)	d 0.46 ( 6.52%)
110.	(0.00127)	R <sub>Y</sub> * ( 3)	C	4	0.0000	-0.0012	0.3773	0.0030
					0.0082	0.0220	-0.5279	-0.1787
					-0.0352	0.5771	0.2878	0.0140
					0.1846	-0.0571	0.0475	0.1566
					-0.0331	0.7373%	p 0.24 ( 17.64%)	d 0.12 ( 8.63%)
111.	(0.00050)	R <sub>Y</sub> * ( 4)	C	4				

					0.0000	0.0020	0.8527	0.1000	0.0134
					0.0094	0.3776	-0.0891	0.0173	-0.1195
					0.0459	-0.0060	0.0905	-0.0291	-0.1190
					0.0146	-0.0798	-0.2211	0.1292	
112.	(0.00042)	RY*( 5)	C	4	s( 0.28%)	p26.27( 7.29%)	d99.99( 92.43%)		
					0.0000	0.0001	0.0523	0.0065	-0.0001
					0.0006	0.0302	-0.0149	0.0021	-0.0899
					0.0469	0.0032	-0.2335	0.0835	-0.0844
					-0.0298	0.7332	-0.3159	-0.5281	
113.	(0.00015)	RY*( 6)	C	4	s( 17.67%)	p 3.71( 65.49%)	d 0.95( 16.84%)		
					0.0000	0.0165	-0.2577	0.3206	-0.0853
					-0.0169	-0.0827	-0.7022	0.0030	-0.1589
					0.3216	-0.0021	0.0560	-0.1510	-0.0736
					-0.0138	-0.0435	-0.3633	0.1700	
114.	(0.00012)	RY*( 7)	C	4	s( 5.73%)	p12.22( 69.98%)	d 4.24( 24.29%)		
					0.0000	0.0095	0.0416	0.2258	-0.0667
					0.0044	-0.1693	-0.2618	-0.0271	0.2486
					-0.6880	0.0099	-0.0976	0.2389	-0.4616
					0.1567	0.0212	0.0147	0.0677	
115.	(0.00008)	RY*( 8)	C	4	s( 15.02%)	p 2.85( 42.76%)	d 2.81( 42.22%)		
116.	(0.00005)	RY*( 9)	C	4	s( 5.25%)	p 2.05( 10.76%)	d16.00( 83.99%)		
117.	(0.00003)	RY*(10)	C	4	s( 0.11%)	p99.99( 92.44%)	d70.37( 7.45%)		
118.	(0.00002)	RY*(11)	C	4	s( 63.60%)	p 0.11( 7.21%)	d 0.46( 29.19%)		
119.	(0.00000)	RY*(12)	C	4	s( 98.34%)	p 0.01( 0.76%)	d 0.01( 0.90%)		
120.	(0.00000)	RY*(13)	C	4	s( 0.03%)	p99.99( 17.85%)	d99.99( 82.12%)		
121.	(0.00001)	RY*(14)	C	4	s( 0.39%)	p56.81( 22.02%)	d99.99( 77.59%)		
122.	(0.00382)	RY*( 1)	C	5	s( 0.01%)	p99.99( 82.81%)	d99.99( 17.18%)		
					0.0000	-0.0001	0.0122	0.0001	0.0008
					0.0012	0.0630	-0.0121	-0.0126	-0.2710
					0.0710	-0.0346	-0.8462	0.1673	0.1364
					0.3882	0.0137	-0.0267	0.0396	
123.	(0.00294)	RY*( 2)	C	5	s( 5.54%)	p15.11( 83.76%)	d 1.93( 10.70%)		
					0.0000	-0.0044	0.2344	0.0205	0.0054
					-0.0239	-0.1021	0.0304	0.0013	0.8377
					0.2019	-0.0010	-0.2778	-0.0773	-0.3019
					0.0837	-0.0330	-0.0807	0.0357	
124.	(0.00131)	RY*( 3)	C	5	s( 14.71%)	p 5.39( 79.38%)	d 0.40( 5.91%)		
					0.0000	-0.0011	0.3828	0.0219	0.0098
					0.0401	-0.7753	-0.3242	0.0179	-0.2271
					-0.1783	-0.0043	0.0228	0.0423	-0.2017
					0.0747	-0.0534	-0.0996	0.0068	
125.	(0.00051)	RY*( 4)	C	5	s( 74.28%)	p 0.25( 18.67%)	d 0.10( 7.06%)		
					0.0000	0.0014	0.8591	0.0675	0.0126
					-0.0033	0.4112	-0.0867	-0.0191	-0.0812
					0.0106	0.0067	0.0541	-0.0037	0.2242
					-0.1214	0.0359	0.0117	0.0645	
126.	(0.00042)	RY*( 5)	C	5	s( 0.13%)	p55.16( 7.07%)	d99.99( 92.81%)		
					0.0000	0.0001	0.0355	0.0045	0.0001
					0.0004	-0.0017	0.0086	-0.0018	0.0817
					-0.0196	-0.0033	0.2385	-0.0813	0.1610
					0.5545	0.6206	-0.2761	-0.3650	
127.	(0.00015)	RY*( 6)	C	5	s( 14.57%)	p 4.54( 66.13%)	d 1.33( 19.31%)		
					0.0000	0.0165	-0.2282	0.2904	-0.0949
					-0.0170	0.0378	-0.7791	0.0052	0.1708
					0.1156	-0.0030	-0.0540	-0.0837	0.3683
					-0.1583	0.0678	-0.1250	0.1100	
128.	(0.00012)	RY*( 7)	C	5	s( 5.98%)	p11.52( 68.94%)	d 4.19( 25.08%)		
					0.0000	0.0098	0.0566	0.2284	-0.0660
					0.0207	-0.2972	0.1994	0.0206	-0.1327
					0.6971	-0.0057	0.0276	-0.2368	0.1661
					-0.0436	0.1924	0.4283	0.0282	
129.	(0.00008)	RY*( 8)	C	5	s( 23.54%)	p 1.92( 45.23%)	d 1.33( 31.24%)		
130.	(0.00005)	RY*( 9)	C	5	s( 10.46%)	p 1.23( 12.89%)	d 7.32( 76.64%)		
131.	(0.00002)	RY*(10)	C	5	s( 0.02%)	p99.99( 94.02%)	d99.99( 5.96%)		
132.	(0.00003)	RY*(11)	C	5	s( 32.44%)	p 0.21( 6.95%)	d 1.87( 60.61%)		
133.	(0.00000)	RY*(12)	C	5	s( 2.06%)	p 8.30( 17.06%)	d39.33( 80.88%)		
134.	(0.00001)	RY*(13)	C	5	s( 18.25%)	p 0.91( 16.54%)	d 3.57( 65.21%)		
135.	(0.00000)	RY*(14)	C	5	s( 98.04%)	p 0.01( 0.73%)	d 0.01( 1.22%)		
136.	(0.00332)	RY*( 1)	B	6	s( 37.85%)	p 1.49( 56.32%)	d 0.15( 5.82%)		
					0.0000	0.0049	0.6124	0.0564	0.0157
					0.0004	-0.7412	-0.0538	0.0042	0.0738

				0.0159	-0.0011	-0.0560	0.0461	-0.1944
				0.0556	0.0461	0.1234	-0.0015	
137.	(0.00186)	RY*( 2)	B 6	s( 15.19%)	p 4.19( 63.73%)	d 1.39( 21.08%)		
				0.0000	-0.0165	0.3807	-0.0803	0.0174
				-0.0056	0.3743	0.3421	0.0069	-0.5877
				0.1332	-0.0069	0.1031	0.0792	-0.3499
				0.1020	0.0871	0.2650	0.0109	
138.	(0.00121)	RY*( 3)	B 6	s( 30.06%)	p 2.28( 68.51%)	d 0.05( 1.44%)		
				0.0000	-0.0062	0.5463	-0.0335	-0.0317
				0.0068	0.5290	-0.2502	-0.0036	0.5350
				0.1413	-0.0022	-0.1895	-0.0223	0.0674
				-0.0221	0.0702	0.0514	0.0421	
139.	(0.00078)	RY*( 4)	B 6	s( 8.17%)	p 9.96( 81.36%)	d 1.28( 10.47%)		
				0.0000	0.0065	0.2809	0.0095	-0.0512
				0.0022	0.0802	-0.3860	-0.0053	-0.2103
				-0.3593	-0.0056	0.6586	-0.2258	0.1220
				-0.0340	-0.0775	-0.2872	0.0134	
140.	(0.00065)	RY*( 5)	B 6	s( 2.66%)	p30.26( 80.62%)	d 6.28( 16.72%)		
				0.0000	-0.0154	-0.0638	0.1492	0.0088
				-0.0014	0.0456	0.4709	0.0123	0.4806
				-0.4576	-0.0046	0.3706	-0.0663	-0.1628
				0.1474	0.1170	0.3242	-0.0119	
141.	(0.00052)	RY*( 6)	B 6	s( 0.80%)	p99.99( 94.12%)	d 6.34( 5.08%)		
				0.0000	-0.0016	-0.0614	-0.0174	0.0627
				0.0011	-0.0959	0.1254	-0.0077	0.1527
				0.7436	0.0018	0.4450	-0.3768	0.1149
				0.1900	0.0024	0.0342	0.0173	
142.	(0.00029)	RY*( 7)	B 6	s( 51.67%)	p 0.20( 10.55%)	d 0.73( 37.78%)		
				0.0000	-0.0012	-0.1268	0.7075	-0.0084
				0.0025	0.0541	-0.2656	-0.0117	-0.0381
				0.1510	-0.0112	0.0638	-0.0585	-0.3310
				-0.4150	0.2552	0.1393	-0.1069	
143.	(0.00027)	RY*( 8)	B 6	s( 17.00%)	p 0.78( 13.31%)	d 4.10( 69.68%)		
				0.0000	0.0018	-0.0837	0.3988	0.0634
				-0.0033	0.0541	-0.3227	0.0034	-0.0975
				-0.0407	0.0188	-0.0840	0.0863	0.0546
				0.7407	-0.1905	0.2285	0.2382	
144.	(0.00015)	RY*( 9)	B 6	s( 34.87%)	p 0.68( 23.65%)	d 1.19( 41.48%)		
				0.0000	-0.0044	0.2550	0.5320	-0.0253
				0.0026	0.0467	0.4593	0.0016	-0.0609
				0.0034	0.0076	-0.1324	-0.0451	0.3642
				-0.0213	-0.3548	-0.3187	-0.2330	
145.	(0.00012)	RY*(10)	B 6	s( 0.45%)	p99.99( 91.05%)	d18.73( 8.50%)		
				0.0000	0.0028	0.0138	0.0492	0.0438
				-0.0010	-0.0063	-0.0106	0.0067	0.0725
				0.1742	0.0032	0.3639	0.8616	0.2376
				-0.0165	0.1408	-0.0334	-0.0854	
146.	(0.00008)	RY*(11)	B 6	s( 2.73%)	p 3.15( 8.60%)	d32.47( 88.67%)		
147.	(0.00004)	RY*(12)	B 6	s( 0.67%)	p 5.07( 3.38%)	d99.99( 95.95%)		
148.	(0.00005)	RY*(13)	B 6	s( 96.49%)	p 0.01( 0.55%)	d 0.03( 2.96%)		
149.	(0.00004)	RY*(14)	B 6	s( 1.48%)	p 2.94( 4.34%)	d63.79( 94.18%)		
150.	(0.01708)	RY*( 1)	C 7	s( 21.80%)	p 3.56( 77.53%)	d 0.03( 0.66%)		
				0.0000	-0.0467	0.4645	0.0057	-0.0072
				0.0266	0.1494	-0.0040	-0.0662	-0.8346
				-0.0335	0.0255	0.2226	0.0000	0.0262
				0.0013	-0.0401	-0.0626	0.0203	
151.	(0.00511)	RY*( 2)	C 7	s( 0.15%)	p77.66( 11.64%)	d99.99( 88.21%)		
				0.0000	0.0026	0.0304	-0.0238	-0.0014
				0.0046	-0.0678	-0.0065	0.0143	-0.0046
				-0.0919	0.0496	-0.1556	-0.2764	-0.0531
				0.1332	-0.7885	0.2475	0.4226	
152.	(0.00299)	RY*( 3)	C 7	s( 8.36%)	p 1.31( 10.92%)	d 9.65( 80.72%)		
				0.0000	0.0053	0.2490	-0.1470	0.0006
				0.0177	0.2050	-0.1096	-0.0140	0.2318
				-0.0070	0.0017	-0.0102	0.0272	0.8003
				-0.1830	-0.1749	-0.3181	0.0383	
153.	(0.00136)	RY*( 4)	C 7	s( 39.69%)	p 0.57( 22.78%)	d 0.95( 37.54%)		
				0.0000	-0.0033	0.6216	-0.1020	-0.0082
				0.0065	-0.3607	0.0440	-0.0501	0.2824
				0.0582	0.0133	-0.0986	-0.0124	-0.3726
				0.0950	-0.0458	-0.4743	-0.0207	

154.	(0.00024)	RY*( 5)	C	7	s( 1.62%)p52.69( 85.48%)d 7.95( 12.90%) 0.0000 -0.0019 0.1245 -0.0177 0.0201 -0.0100 0.8694 -0.0990 -0.0140 0.1608 0.0980 0.0085 -0.2095 -0.0974 -0.3209 0.1286 -0.0195 -0.0654 -0.0691
155.	(0.00022)	RY*( 6)	C	7	s( 36.18%)p 0.51( 18.32%)d 1.26( 45.50%) 0.0000 0.0258 0.5202 0.2935 -0.0665 0.0039 0.0284 0.0072 -0.0248 0.2500 -0.3224 0.0064 -0.0323 0.1189 0.0839 -0.0533 0.2475 0.6089 0.1145
156.	(0.00013)	RY*( 7)	C	7	s( 8.88%)p 9.43( 83.73%)d 0.83( 7.39%) 0.0000 -0.0074 0.1253 0.2671 0.0418 0.0042 -0.0672 -0.3603 -0.0066 0.0921 0.7867 0.0027 0.2746 -0.0044 -0.0066 -0.1278 -0.1105 0.2106 -0.0301
157.	(0.00009)	RY*( 8)	C	7	s( 15.82%)p 4.59( 72.62%)d 0.73( 11.55%)
158.	(0.00006)	RY*( 9)	C	7	s( 38.71%)p 0.69( 26.63%)d 0.90( 34.66%)
159.	(0.00006)	RY*(10)	C	7	s( 13.70%)p 5.87( 80.43%)d 0.43( 5.87%)
160.	(0.00004)	RY*(11)	C	7	s( 3.24%)p28.32( 91.81%)d 1.53( 4.95%)
161.	(0.00000)	RY*(12)	C	7	s( 99.43%)p 0.00( 0.43%)d 0.00( 0.14%)
162.	(0.00001)	RY*(13)	C	7	s( 0.27%)p34.84( 9.44%)d99.99( 90.29%)
163.	(0.00001)	RY*(14)	C	7	s( 11.63%)p 0.78( 9.12%)d 6.81( 79.25%)
164.	(0.00547)	RY*( 1)	O	8	s( 1.07%)p90.26( 96.41%)d 2.36( 2.53%) 0.0000 0.0026 0.1033 -0.0036 0.0002 0.0135 -0.9595 -0.0114 -0.0034 -0.1501 -0.0032 -0.0037 0.1430 0.0028 -0.1495 0.0365 0.0237 0.0318 -0.0022
165.	(0.00304)	RY*( 2)	O	8	s( 0.57%)p99.99( 98.11%)d 2.30( 1.32%) 0.0000 0.0016 0.0754 0.0063 0.0009 -0.0038 -0.0858 0.0023 -0.0069 -0.2855 0.0077 -0.0170 -0.9443 0.0056 -0.0167 0.0291 -0.0961 0.0285 0.0446
166.	(0.00190)	RY*( 3)	O	8	s( 89.46%)p 0.12( 10.48%)d 0.00( 0.05%) 0.0000 -0.0033 0.9423 0.0814 0.0032 0.0006 0.0523 -0.0259 -0.0122 0.2845 0.1361 0.0037 -0.0166 -0.0384 0.0078 -0.0067 0.0103 -0.0109 -0.0145
167.	(0.00029)	RY*( 4)	O	8	s( 13.42%)p 6.38( 85.59%)d 0.07( 1.00%) 0.0000 -0.0240 -0.2319 0.2824 -0.0057 -0.0031 -0.1914 0.0476 0.0293 0.8328 -0.2269 -0.0078 -0.2501 0.0919 -0.0304 -0.0272 -0.0602 -0.0148 -0.0668
168.	(0.00005)	RY*( 5)	O	8	s( 38.58%)p 0.65( 25.03%)d 0.94( 36.39%)
169.	(0.00000)	RY*( 6)	O	8	s( 99.91%)p 0.00( 0.04%)d 0.00( 0.05%)
170.	(0.00001)	RY*( 7)	O	8	s( 15.64%)p 4.92( 76.91%)d 0.48( 7.45%)
171.	(0.00001)	RY*( 8)	O	8	s( 1.41%)p69.37( 97.74%)d 0.60( 0.85%)
172.	(0.00000)	RY*( 9)	O	8	s( 1.13%)p87.21( 98.38%)d 0.43( 0.49%)
173.	(0.00000)	RY*(10)	O	8	s( 0.71%)p 4.54( 3.20%)d99.99( 96.09%)
174.	(0.00000)	RY*(11)	O	8	s( 0.22%)p 1.61( 0.35%)d99.99( 99.44%)
175.	(0.00000)	RY*(12)	O	8	s( 0.95%)p 2.67( 2.53%)d99.99( 96.53%)
176.	(0.00001)	RY*(13)	O	8	s( 36.81%)p 0.12( 4.38%)d 1.60( 58.81%)
177.	(0.00000)	RY*(14)	O	8	s( 0.17%)p 6.48( 1.13%)d99.99( 98.70%)
178.	(0.00172)	RY*( 1)	C	9	s( 3.14%)p25.22( 79.23%)d 5.61( 17.63%) 0.0000 -0.0016 0.1721 0.0425 0.0017 0.0129 0.5567 0.0152 0.0192 -0.5724 -0.0583 -0.0147 -0.3423 0.1822 -0.2019 0.0860 0.2772 -0.1227 -0.1905
179.	(0.00162)	RY*( 2)	C	9	s( 0.60%)p99.99( 79.22%)d33.84( 20.18%) 0.0000 0.0012 0.0516 0.0574 0.0005 0.0138 0.6512 0.1104 0.0106 0.1629 -0.1650 0.0046 0.5404 -0.0995 -0.2191 0.0618 -0.2996 0.1263 0.2105
180.	(0.00121)	RY*( 3)	C	9	s( 7.82%)p11.01( 86.15%)d 0.77( 6.03%) 0.0000 -0.0046 0.2797 -0.0014 -0.0029 -0.0055 -0.3172 -0.1801 0.0318 -0.7012 -0.0842 -0.0075 0.4724 -0.0737 0.1126 -0.0659 -0.1386 0.0436 0.1488
181.	(0.00034)	RY*( 4)	C	9	s( 45.00%)p 1.11( 49.83%)d 0.12( 5.18%) 0.0000 0.0053 0.6371 0.2099 0.0035 -0.0020 -0.1648 0.1788 -0.0005 0.2588 -0.5430 -0.0010 -0.0625 0.2710 0.0279

182.	(0.00012)	RY*( 5)	C	9	0.0166 0.1354 0.1782 -0.0248 s( 5.77%)p13.45( 77.63%)d 2.88( 16.60%) 0.0000 0.0101 -0.1584 0.1640 -0.0751 -0.0093 0.0968 -0.7531 0.0037 0.1441 -0.3580 -0.0033 0.0637 0.2160 0.1114 -0.0403 -0.0258 -0.3869 -0.0402
183.	(0.00006)	RY*( 6)	C	9	s( 41.89%)p 1.32( 55.47%)d 0.06( 2.64%)
184.	(0.00005)	RY*( 7)	C	9	s( 1.62%)p59.04( 95.41%)d 1.84( 2.98%)
185.	(0.00005)	RY*( 8)	C	9	s( 0.40%)p80.67( 32.63%)d99.99( 66.96%)
186.	(0.00003)	RY*( 9)	C	9	s( 7.25%)p 0.87( 6.33%)d11.93( 86.42%)
187.	(0.00001)	RY*(10)	C	9	s( 0.15%)p32.11( 4.79%)d99.99( 95.06%)
188.	(0.00002)	RY*(11)	C	9	s( 78.66%)p 0.16( 12.60%)d 0.11( 8.75%)
189.	(0.00001)	RY*(12)	C	9	s( 1.10%)p13.27( 14.63%)d76.47( 84.27%)
190.	(0.00000)	RY*(13)	C	9	s( 98.68%)p 0.01( 0.94%)d 0.00( 0.38%)
191.	(0.00000)	RY*(14)	C	9	s( 7.87%)p 0.69( 5.41%)d11.03( 86.73%)
192.	(0.00214)	RY*( 1)	C	10	s( 0.17%)p99.99( 76.15%)d99.99( 23.68%) 0.0000 0.0000 0.0402 -0.0069 0.0009 -0.0012 -0.0369 -0.0192 -0.0048 -0.2263 0.0899 -0.0139 -0.8091 0.2138 -0.0855 -0.2547 -0.3266 0.1249 0.2058
193.	(0.00162)	RY*( 2)	C	10	s( 1.75%)p49.11( 86.00%)d 6.99( 12.25%) 0.0000 0.0023 0.1041 0.0816 0.0024 0.0060 0.7763 0.2212 -0.0189 -0.4343 0.0743 0.0056 0.1177 0.0057 0.0989 -0.0502 0.0699 0.3240 -0.0177
194.	(0.00081)	RY*( 3)	C	10	s( 32.87%)p 2.01( 66.05%)d 0.03( 1.08%) 0.0000 -0.0010 0.5548 0.1443 -0.0067 -0.0220 0.2707 0.0219 -0.0245 0.6079 0.3992 0.0091 -0.1868 -0.1479 -0.0129 0.0305 0.0453 -0.0857 0.0169
195.	(0.00022)	RY*( 4)	C	10	s( 31.16%)p 1.68( 52.28%)d 0.53( 16.56%) 0.0000 -0.0014 0.5554 -0.0347 0.0444 0.0124 -0.3512 0.5496 0.0024 -0.2191 -0.1832 0.0001 0.0043 0.1251 -0.2752 0.2137 0.1626 0.1193 -0.0598
196.	(0.00013)	RY*( 5)	C	10	s( 2.50%)p15.22( 38.09%)d23.74( 59.41%) 0.0000 -0.0016 0.1335 -0.0837 0.0147 -0.0039 0.0445 -0.3926 -0.0019 -0.2833 -0.0346 0.0066 -0.3773 -0.0298 0.2124 0.3448 0.5145 -0.2354 -0.3316
197.	(0.00009)	RY*( 6)	C	10	s( 33.85%)p 1.60( 54.13%)d 0.36( 12.03%)
198.	(0.00005)	RY*( 7)	C	10	s( 20.21%)p 3.10( 62.68%)d 0.85( 17.12%)
199.	(0.00003)	RY*( 8)	C	10	s( 7.68%)p 2.48( 19.06%)d 9.54( 73.26%)
200.	(0.00003)	RY*( 9)	C	10	s( 2.88%)p25.99( 74.77%)d 7.77( 22.36%)
201.	(0.00001)	RY*(10)	C	10	s( 0.13%)p99.99( 13.18%)d99.99( 86.69%)
202.	(0.00002)	RY*(11)	C	10	s( 63.12%)p 0.55( 34.94%)d 0.03( 1.93%)
203.	(0.00001)	RY*(12)	C	10	s( 2.50%)p 5.59( 13.98%)d33.39( 83.52%)
204.	(0.00000)	RY*(13)	C	10	s( 98.72%)p 0.01( 0.71%)d 0.01( 0.56%)
205.	(0.00000)	RY*(14)	C	10	s( 2.41%)p 3.43( 8.24%)d37.14( 89.35%)
206.	(0.00346)	RY*( 1)	B	11	s( 11.83%)p 7.36( 87.09%)d 0.09( 1.07%) 0.0000 -0.0058 0.2570 -0.2273 -0.0246 0.0248 -0.7795 -0.3396 0.0000 -0.2896 -0.0731 0.0042 0.2397 0.0268 -0.0890 0.0410 0.0184 0.0223 -0.0176
207.	(0.00204)	RY*( 2)	B	11	s( 27.74%)p 2.17( 60.32%)d 0.43( 11.93%) 0.0000 -0.0023 0.4497 0.2717 -0.0370 0.0074 0.1782 -0.2070 0.0039 -0.5236 0.2889 -0.0035 -0.3731 0.1781 0.2968 -0.1256 -0.0329 0.0766 0.0922
208.	(0.00147)	RY*( 3)	B	11	s( 46.57%)p 0.99( 45.99%)d 0.16( 7.45%) 0.0000 -0.0037 0.6773 0.0820 -0.0119 -0.0028 -0.0310 -0.0612 0.0178 0.6183 -0.0967 0.0030 -0.2269 0.1081 -0.2636 0.0129 -0.0102 -0.0637 -0.0256
209.	(0.00103)	RY*( 4)	B	11	s( 14.00%)p 5.07( 71.07%)d 1.07( 14.92%) 0.0000 0.0009 0.3711 0.0335 -0.0347 0.0040 0.2565 0.0753 0.0006 0.0197 0.0996 0.0008 0.7661 -0.2050 0.1568 -0.3481 -0.0380 0.0401 0.0209
210.	(0.00075)	RY*( 5)	B	11	s( 51.76%)p 0.64( 33.35%)d 0.29( 14.89%) 0.0000 -0.0184 -0.3023 0.6513 0.0411

					-0.0009	-0.2501	-0.3709	0.0028	0.3178
					-0.0546	0.0075	0.0985	0.1399	0.2395
					-0.2593	-0.0798	0.0763	0.1102	
211.	(0.00049)	RY*( 6)	B	11	s( 2.47%)	p33.87( 83.55%)	d 5.67( 13.99%)		
					0.0000	0.0123	-0.0764	0.1318	-0.0362
					0.0040	-0.2765	0.3574	-0.0031	0.0802
					0.7827	0.0124	0.0279	0.1060	-0.3144
					-0.1097	0.1361	0.0445	0.0920	
212.	(0.00035)	RY*( 7)	B	11	s( 12.07%)	p 3.31( 40.01%)	d 3.97( 47.92%)		
					0.0000	0.0046	0.1752	0.2890	0.0804
					0.0059	-0.2775	0.5208	-0.0074	0.0115
					-0.1656	-0.0194	0.0000	-0.1543	0.4781
					0.3308	0.3738	-0.0039	-0.0386	
213.	(0.00024)	RY*( 8)	B	11	s( 15.61%)	p 3.25( 50.70%)	d 2.16( 33.69%)		
					0.0000	-0.0041	0.0072	0.2799	-0.2788
					-0.0042	0.1102	-0.3454	-0.0156	0.0021
					0.2300	-0.0100	0.0676	-0.5637	-0.1647
					0.5445	-0.0084	0.0676	-0.0932	
214.	(0.00016)	RY*( 9)	B	11	s( 17.89%)	p 1.22( 21.79%)	d 3.37( 60.32%)		
					0.0000	0.0150	0.0337	0.4202	-0.0321
					0.0036	-0.0671	0.2552	-0.0145	-0.3055
					-0.2224	0.0073	0.0270	-0.0666	-0.3581
					-0.0968	-0.3311	-0.5836	-0.1239	
215.	(0.00012)	RY*(10)	B	11	s( 7.35%)	p 7.25( 53.26%)	d 5.36( 39.40%)		
					0.0000	0.0016	0.0054	0.2455	-0.1146
					0.0034	0.1932	0.0099	0.0110	-0.1715
					-0.1936	-0.0104	0.2937	0.5846	-0.3276
					0.2678	0.2879	0.3093	-0.1907	
216.	(0.00009)	RY*(11)	B	11	s( 4.46%)	p 3.01( 13.43%)	d18.43( 82.11%)		
217.	(0.00007)	RY*(12)	B	11	s( 83.49%)	p 0.05( 3.92%)	d 0.15( 12.59%)		
218.	(0.00004)	RY*(13)	B	11	s( 3.84%)	p 8.39( 32.18%)	d16.68( 63.98%)		
219.	(0.00004)	RY*(14)	B	11	s( 1.02%)	p 3.43( 3.49%)	d93.87( 95.49%)		
220.	(0.00478)	RY*( 1)	C	12	s( 7.30%)	p11.43( 83.47%)	d 1.27( 9.24%)		
					0.0000	0.0187	0.2678	0.0305	-0.0001
					0.0331	0.9062	-0.0561	0.0218	-0.0734
					-0.0211	-0.0102	-0.0187	-0.0498	0.1015
					-0.0607	0.0933	-0.2162	0.1514	
221.	(0.00303)	RY*( 2)	C	12	s( 15.51%)	p 3.18( 49.39%)	d 2.26( 35.10%)		
					0.0000	-0.0109	0.3578	-0.1642	0.0036
					-0.0055	-0.2169	0.0473	0.0333	-0.3585
					-0.1380	-0.0230	0.4832	-0.2488	0.4840
					-0.2454	-0.0967	0.0536	0.2105	
222.	(0.00209)	RY*( 3)	C	12	s( 35.27%)	p 1.64( 58.01%)	d 0.19( 6.71%)		
					0.0000	-0.0069	0.5778	-0.1374	-0.0012
					0.0137	-0.1118	0.2574	0.0033	-0.3932
					0.2261	0.0147	-0.5247	0.1410	-0.1966
					0.0208	-0.0954	0.1369	-0.0142	
223.	(0.00185)	RY*( 4)	C	12	s( 17.83%)	p 2.85( 50.75%)	d 1.76( 31.42%)		
					0.0000	-0.0012	0.4077	-0.1097	-0.0006
					0.0172	-0.0391	0.2485	-0.0090	0.4621
					-0.3761	0.0237	-0.0070	-0.2970	0.0555
					0.3230	-0.0854	-0.1778	-0.4098	
224.	(0.00146)	RY*( 5)	C	12	s( 12.10%)	p 6.22( 75.33%)	d 1.04( 12.57%)		
					0.0000	-0.0003	0.3386	-0.0798	-0.0020
					0.0139	0.0120	0.0964	-0.0284	0.5285
					0.4380	-0.0290	0.4225	0.3040	-0.1798
					-0.0569	-0.0017	0.1953	0.2279	
225.	(0.00092)	RY*( 6)	C	12	s( 0.04%)	p99.99( 20.61%)	d99.99( 79.35%)		
					0.0000	-0.0001	0.0050	0.0195	-0.0029
					0.0009	0.0231	0.0200	-0.0129	-0.1809
					0.2632	-0.0100	0.2699	0.1734	-0.1167
					-0.3749	-0.1677	-0.4140	-0.6632	
226.	(0.00056)	RY*( 7)	C	12	s( 0.25%)	p99.99( 55.27%)	d99.99( 44.48%)		
					0.0000	-0.0013	0.0020	0.0497	-0.0014
					0.0040	0.0706	-0.0856	0.0030	-0.3155
					0.3265	0.0026	0.3448	-0.4641	-0.3332
					0.5155	0.1614	0.1549	-0.1344	
227.	(0.00045)	RY*( 8)	C	12	s( 74.61%)	p 0.32( 23.95%)	d 0.02( 1.44%)		
					0.0000	0.0005	0.0326	0.8632	0.0018
					0.0114	-0.0061	0.4828	0.0033	-0.0320
					-0.0145	-0.0013	0.0631	-0.0315	0.0521



228.	(0.00016)	RY*( 9)	C	12	-0.0458 -0.0478 0.0742 0.0428
					s( 25.43%)p 1.45( 36.78%)d 1.49( 37.79%)
					0.0000 -0.0175 0.3761 0.3344 0.0282
					0.0092 -0.2945 -0.5087 -0.0007 0.0013
					-0.0632 0.0018 -0.0207 0.1333 -0.0454
					0.0653 0.4575 -0.3930 0.0885
229.	(0.00008)	RY*(10)	C	12	s( 9.13%)p 3.87( 35.30%)d 6.08( 55.56%)
230.	(0.00007)	RY*(11)	C	12	s( 0.54%)p46.70( 25.00%)d99.99( 74.46%)
231.	(0.00005)	RY*(12)	C	12	s( 0.55%)p99.99( 66.02%)d60.45( 33.42%)
232.	(0.00003)	RY*(13)	C	12	s( 4.96%)p 4.05( 20.09%)d15.10( 74.95%)
233.	(0.00000)	RY*(14)	C	12	s( 96.45%)p 0.00( 0.35%)d 0.03( 3.20%)
234.	(0.00409)	RY*( 1)	N	13	s( 15.53%)p 4.99( 77.45%)d 0.45( 7.03%)
					0.0000 -0.0086 0.3939 -0.0005 -0.0006
					0.0032 -0.0022 -0.0481 0.0088 -0.1283
					0.0572 0.0084 -0.8673 -0.0124 -0.1753
					-0.0700 -0.0923 0.1530 -0.0521
235.	(0.00366)	RY*( 2)	N	13	s( 0.47%)p99.99( 92.20%)d15.43( 7.32%)
					0.0000 -0.0070 0.0678 -0.0098 0.0008
					0.0039 -0.2112 -0.0354 0.0082 -0.9039
					0.0051 0.0038 0.2269 0.0863 -0.0043
					-0.1537 -0.1291 0.1641 -0.0775
236.	(0.00184)	RY*( 3)	N	13	s( 2.58%)p30.69( 79.23%)d 7.05( 18.19%)
					0.0000 0.0035 0.1315 0.0923 -0.0005
					-0.0008 -0.8516 -0.0049 0.0017 0.2567
					0.0219 0.0029 0.0236 -0.0035 0.2578
					0.1666 -0.1560 0.2385 -0.0803
237.	(0.00084)	RY*( 4)	N	13	s( 75.40%)p 0.24( 17.90%)d 0.09( 6.71%)
					0.0000 0.0074 0.8577 0.1353 -0.0024
					-0.0019 0.1808 -0.0432 0.0036 0.0743
					0.0176 0.0001 0.3719 -0.0160 -0.0783
					0.1986 -0.0414 -0.1099 -0.0878
238.	(0.00061)	RY*( 5)	N	13	s( 5.14%)p 1.52( 7.81%)d16.93( 87.05%)
					0.0000 0.0013 0.2266 0.0079 0.0017
					0.0001 0.0684 0.0268 -0.0039 0.0548
					-0.1565 0.0053 -0.0124 0.2122 0.5227
					-0.4895 0.0357 0.0759 0.5921
239.	(0.00045)	RY*( 6)	N	13	s( 0.20%)p26.19( 5.20%)d99.99( 94.60%)
					0.0000 0.0002 0.0190 0.0403 -0.0001
					0.0012 0.0149 -0.0247 0.0035 0.0617
					0.1276 -0.0046 -0.0364 -0.1725 0.3576
					-0.5038 -0.2130 -0.4209 -0.5847
240.	(0.00021)	RY*( 7)	N	13	s( 8.62%)p 2.08( 17.91%)d 8.52( 73.47%)
					0.0000 -0.0054 -0.0989 0.2762 0.0105
					0.0264 0.3287 -0.0844 -0.0103 -0.1653
					-0.1053 -0.0118 -0.1478 -0.0518 0.6355
					0.5270 -0.0886 0.1619 -0.1378
241.	(0.00013)	RY*( 8)	N	13	s( 0.31%)p63.70( 19.76%)d99.99( 79.93%)
					0.0000 -0.0087 0.0521 0.0029 0.0173
					-0.0111 -0.2781 -0.2161 -0.0066 -0.2134
					-0.0331 -0.0033 -0.1579 -0.0433 0.1193
					0.2175 0.5145 -0.6655 0.1738
242.	(0.00011)	RY*( 9)	N	13	s( 6.87%)p12.97( 89.12%)d 0.58( 4.01%)
					0.0000 -0.0017 -0.0077 0.2614 -0.0166
					0.0063 -0.0121 0.7259 0.0050 -0.0613
					0.4736 0.0016 -0.0601 0.3638 0.0421
					0.0939 0.0459 -0.1636 0.0260
243.	(0.00009)	RY*(10)	N	13	s( 68.16%)p 0.32( 21.68%)d 0.15( 10.17%)
244.	(0.00005)	RY*(11)	N	13	s( 15.65%)p 5.12( 80.10%)d 0.27( 4.25%)
245.	(0.00002)	RY*(12)	N	13	s( 2.15%)p 1.80( 3.88%)d43.70( 93.97%)
246.	(0.00001)	RY*(13)	N	13	s( 0.34%)p99.99( 87.73%)d34.74( 11.93%)
247.	(0.00000)	RY*(14)	N	13	s( 98.65%)p 0.00( 0.13%)d 0.01( 1.23%)
248.	(0.00396)	RY*( 1)	C	14	s( 1.08%)p74.34( 79.97%)d17.62( 18.95%)
					0.0000 -0.0015 0.1019 -0.0187 0.0049
					0.0080 0.1653 -0.0150 -0.0210 -0.7036
					0.1019 0.0287 0.4928 -0.1501 -0.2797
					0.2766 0.0537 0.1574 0.0845
249.	(0.00302)	RY*( 2)	C	14	s( 5.56%)p15.14( 84.13%)d 1.86( 10.32%)
					0.0000 -0.0043 0.2353 0.0117 0.0065
					0.0224 0.3249 0.0399 0.0126 -0.4355
					-0.1825 -0.0021 -0.7070 -0.1027 -0.1423
					-0.2678 -0.0824 0.0601 -0.0284

250.	(0.00133)	RY*( 3)	C	14	s( 13.92%)p 5.73( 79.71%)d 0.46( 6.38%) 0.0000 -0.0010 0.3730 -0.0012 0.0058 -0.0304 0.6761 0.2577 -0.0262 0.3954 0.2038 -0.0181 0.2370 0.1327 -0.1824 -0.1646 -0.0070 0.0574 0.0082
251.	(0.00055)	RY*( 4)	C	14	s( 66.04%)p 0.29( 18.90%)d 0.23( 15.06%) 0.0000 0.0024 0.8081 0.0848 0.0134 -0.0040 -0.3972 0.1299 0.0136 0.0158 0.0663 0.0141 -0.0844 0.0470 0.1582 0.2533 0.0366 -0.0522 0.2393
252.	(0.00046)	RY*( 5)	C	14	s( 4.31%)p 2.22( 9.58%)d19.97( 86.10%) 0.0000 0.0010 0.2065 0.0215 0.0023 -0.0020 -0.0559 0.0220 0.0048 -0.2043 0.0753 0.0015 0.2114 -0.0105 0.1904 -0.2443 -0.1695 -0.5064 -0.6928
253.	(0.00015)	RY*( 6)	C	14	s( 24.02%)p 2.32( 55.64%)d 0.85( 20.34%) 0.0000 0.0140 -0.2968 0.3842 -0.0656 0.0138 0.1112 0.6819 0.0005 -0.1390 0.1927 -0.0026 -0.1457 0.0345 0.1823 0.2665 0.0579 -0.2905 0.1071
254.	(0.00013)	RY*( 7)	C	14	s( 11.38%)p 6.27( 71.38%)d 1.52( 17.24%) 0.0000 0.0094 0.0795 0.3229 -0.0563 -0.0097 0.1763 0.0389 -0.0186 0.1600 -0.6227 -0.0149 0.1612 -0.4910 0.2429 0.2036 -0.1961 0.1502 -0.1046
255.	(0.00007)	RY*( 8)	C	14	s( 8.12%)p 5.40( 43.79%)d 5.93( 48.09%)
256.	(0.00005)	RY*( 9)	C	14	s( 9.30%)p 1.21( 11.24%)d 8.54( 79.46%)
257.	(0.00003)	RY*(10)	C	14	s( 0.07%)p99.99( 94.38%)d81.97( 5.55%)
258.	(0.00003)	RY*(11)	C	14	s( 56.19%)p 0.19( 10.47%)d 0.59( 33.35%)
259.	(0.00001)	RY*(12)	C	14	s( 0.22%)p69.30( 15.32%)d99.99( 84.46%)
260.	(0.00001)	RY*(13)	C	14	s( 1.59%)p15.52( 24.62%)d46.51( 73.79%)
261.	(0.00000)	RY*(14)	C	14	s( 98.27%)p 0.01( 1.03%)d 0.01( 0.70%)
262.	(0.00456)	RY*( 1)	C	15	s( 0.06%)p99.99( 84.74%)d99.99( 15.20%) 0.0000 -0.0001 0.0248 0.0019 0.0009 0.0008 -0.1178 0.0332 0.0238 0.6525 -0.1038 -0.0310 -0.6161 0.1216 0.2592 -0.2664 -0.0195 -0.0053 0.1160
263.	(0.00292)	RY*( 2)	C	15	s( 5.57%)p15.13( 84.28%)d 1.82( 10.15%) 0.0000 -0.0049 0.2353 0.0167 0.0054 0.0228 0.3157 0.0379 -0.0051 0.5972 0.1973 -0.0049 0.5664 0.1571 0.2121 0.2196 -0.0597 0.0363 -0.0583
264.	(0.00130)	RY*( 3)	C	15	s( 15.32%)p 5.11( 78.29%)d 0.42( 6.38%) 0.0000 -0.0006 0.3913 -0.0039 0.0090 -0.0339 0.6853 0.2913 0.0199 -0.2444 -0.1747 0.0200 -0.3195 -0.1847 0.2232 0.1170 0.0058 0.0029 0.0158
265.	(0.00054)	RY*( 4)	C	15	s( 69.32%)p 0.28( 19.45%)d 0.16( 11.23%) 0.0000 0.0026 0.8290 0.0757 0.0118 -0.0005 -0.4137 0.0962 -0.0162 -0.0467 -0.0131 -0.0134 0.0991 -0.0384 -0.1841 -0.1652 -0.0159 -0.0603 0.2173
266.	(0.00044)	RY*( 5)	C	15	s( 1.70%)p 4.50( 7.63%)d53.46( 90.67%) 0.0000 0.0013 0.1216 0.0463 0.0051 0.0002 -0.0668 0.0911 -0.0037 0.1521 -0.0787 0.0013 -0.1844 0.0145 -0.3401 0.2432 -0.0739 -0.3993 -0.7530
267.	(0.00017)	RY*( 6)	C	15	s( 22.40%)p 2.49( 55.88%)d 0.97( 21.72%) 0.0000 0.0143 -0.2673 0.3830 -0.0754 0.0133 0.0740 0.7191 0.0041 0.1256 -0.0150 0.0002 0.1333 -0.0465 -0.3171 -0.2006 0.0784 -0.1616 0.2101
268.	(0.00012)	RY*( 7)	C	15	s( 6.83%)p 9.96( 68.07%)d 3.67( 25.10%) 0.0000 0.0083 0.0901 0.2390 -0.0550 -0.0162 0.2424 -0.0900 0.0166 -0.1565 0.5516 0.0189 -0.1921 0.4972 -0.2235 -0.2898 -0.2461 0.2080 -0.1150
269.	(0.00005)	RY*( 8)	C	15	s( 12.72%)p 1.12( 14.29%)d 5.74( 72.99%)
270.	(0.00006)	RY*( 9)	C	15	s( 11.75%)p 4.17( 48.97%)d 3.34( 39.28%)
271.	(0.00002)	RY*(10)	C	15	s( 0.83%)p99.99( 98.49%)d 0.81( 0.68%)
272.	(0.00002)	RY*(11)	C	15	s( 18.75%)p 0.65( 12.21%)d 3.68( 69.04%)

273.	(0.00001)	RY*(12)	C	15	s( 31.58%)p 0.54( 17.09%)d 1.62( 51.32%)
274.	(0.00000)	RY*(13)	C	15	s( 5.95%)p 1.62( 9.67%)d14.17( 84.38%)
275.	(0.00000)	RY*(14)	C	15	s( 97.25%)p 0.01( 1.08%)d 0.02( 1.67%)
276.	(0.00393)	RY*( 1)	N	16	s( 13.65%)p 5.54( 75.59%)d 0.79( 10.76%) 0.0000 -0.0097 0.3692 0.0083 -0.0001 0.0042 -0.1302 -0.0464 -0.0065 0.2987 -0.0685 -0.0126 0.8012 -0.0271 0.1958 0.1302 -0.1394 0.1617 -0.0819
277.	(0.00325)	RY*( 2)	N	16	s( 0.19%)p99.99( 96.72%)d16.38( 3.09%) 0.0000 0.0056 -0.0147 0.0405 0.0005 -0.0044 0.0057 0.0023 0.0105 -0.8946 -0.0046 -0.0034 0.3997 0.0828 -0.0549 -0.1341 0.0134 -0.0496 0.0852
278.	(0.00201)	RY*( 3)	N	16	s( 0.29%)p99.99( 81.69%)d63.13( 18.02%) 0.0000 0.0004 -0.0370 0.0385 -0.0008 -0.0005 -0.8902 -0.0028 -0.0025 -0.0601 -0.0189 -0.0016 -0.1430 -0.0076 -0.1057 -0.2228 -0.1766 0.2452 -0.1675
279.	(0.00068)	RY*( 4)	N	16	s( 28.65%)p 0.41( 11.72%)d 2.08( 59.63%) 0.0000 0.0063 0.5241 0.1084 -0.0030 0.0019 0.0111 -0.0040 -0.0014 -0.1371 0.1540 -0.0028 -0.2163 -0.1664 -0.2969 0.3673 -0.0123 0.4374 0.4264
280.	(0.00054)	RY*( 5)	N	16	s( 52.19%)p 0.23( 12.15%)d 0.68( 35.66%) 0.0000 0.0071 0.7028 0.1670 -0.0041 -0.0078 -0.0001 -0.0008 -0.0072 -0.1098 -0.1257 -0.0046 -0.2923 0.0896 0.3203 -0.2230 -0.1041 -0.3958 -0.1918
281.	(0.00042)	RY*( 6)	N	16	s( 0.75%)p 6.18( 4.64%)d99.99( 94.61%) 0.0000 0.0002 0.0786 0.0365 0.0023 0.0016 -0.0077 -0.0141 -0.0037 -0.0614 -0.1451 0.0010 0.0195 0.1447 -0.5513 0.4886 0.0421 -0.2055 -0.5995
282.	(0.00017)	RY*( 7)	N	16	s( 11.84%)p 1.61( 19.04%)d 5.84( 69.12%) 0.0000 -0.0013 0.0594 0.3388 0.0094 0.0234 0.3319 -0.1047 0.0134 0.1518 0.0289 0.0079 0.0689 0.1997 -0.4549 -0.5855 -0.2364 0.2696 -0.1133
283.	(0.00013)	RY*( 8)	N	16	s( 2.34%)p23.55( 55.08%)d18.21( 42.58%) 0.0000 -0.0028 0.0455 0.1433 0.0276 -0.0146 -0.2461 -0.5000 0.0077 0.1565 0.2764 0.0073 0.1080 0.3569 -0.1835 -0.0171 0.3474 -0.3871 0.3483
284.	(0.00012)	RY*( 9)	N	16	s( 0.97%)p56.19( 54.25%)d46.38( 44.78%) 0.0000 -0.0076 0.0880 0.0430 -0.0009 0.0023 -0.1182 0.4777 0.0009 0.1390 -0.3792 -0.0003 0.1409 -0.3427 -0.3652 -0.2334 0.3037 -0.3036 0.2749
285.	(0.00008)	RY*(10)	N	16	s( 63.06%)p 0.42( 26.70%)d 0.16( 10.24%)
286.	(0.00005)	RY*(11)	N	16	s( 23.91%)p 2.98( 71.38%)d 0.20( 4.71%)
287.	(0.00001)	RY*(12)	N	16	s( 0.83%)p99.99( 86.50%)d15.27( 12.67%)
288.	(0.00002)	RY*(13)	N	16	s( 3.19%)p 1.36( 4.34%)d29.00( 92.48%)
289.	(0.00000)	RY*(14)	N	16	s( 98.20%)p 0.00( 0.28%)d 0.02( 1.52%)
290.	(0.00170)	RY*( 1)	C	17	s( 0.35%)p99.99( 68.28%)d89.00( 31.37%) 0.0000 -0.0013 0.0439 -0.0399 0.0028 -0.0024 0.0907 -0.0565 -0.0086 -0.4943 0.1221 0.0176 0.6155 -0.1810 0.0675 -0.1781 -0.1329 -0.2627 -0.4368
291.	(0.00162)	RY*( 2)	C	17	s( 1.01%)p85.75( 86.70%)d12.16( 12.29%) 0.0000 0.0020 0.0783 0.0630 -0.0016 -0.0090 -0.8656 -0.1723 0.0046 0.1535 -0.0881 0.0111 0.2309 -0.0560 0.2347 0.1610 -0.1031 0.1503 -0.0932
292.	(0.00084)	RY*( 3)	C	17	s( 37.13%)p 1.68( 62.43%)d 0.01( 0.44%) 0.0000 -0.0027 0.6050 0.0723 -0.0065 0.0099 -0.1096 -0.0669 0.0278 -0.5391 -0.2680 0.0190 -0.4451 -0.2146 -0.0401 -0.0124 -0.0327 0.0174 0.0355
293.	(0.00024)	RY*( 4)	C	17	s( 27.05%)p 1.63( 43.96%)d 1.07( 28.98%) 0.0000 0.0025 0.5114 0.0906 0.0284 0.0033 0.1506 0.0130 -0.0106 0.6244

					-0.0322	-0.0024	0.0039	-0.1604	-0.0290
					-0.3675	-0.1493	-0.0308	-0.3615	
294.	(0.00014)	RY*( 5)	C	17	s( 15.69%)	p 2.40( 37.61%)	d 2.97( 46.69%)		
					0.0000	-0.0037	0.3886	-0.0537	0.0551
					-0.0019	0.2020	-0.2770	-0.0058	-0.0180
					0.0689	-0.0074	0.4719	0.1752	-0.2348
					0.1233	0.0016	0.5211	0.3536	
295.	(0.00009)	RY*( 6)	C	17	s( 2.05%)	p41.01( 83.93%)	d 6.85( 14.02%)		
296.	(0.00006)	RY*( 7)	C	17	s( 22.62%)	p 2.89( 65.32%)	d 0.53( 12.06%)		
297.	(0.00004)	RY*( 8)	C	17	s( 2.83%)	p27.64( 78.36%)	d 6.63( 18.80%)		
298.	(0.00003)	RY*( 9)	C	17	s( 5.39%)	p 2.89( 15.58%)	d14.67( 79.03%)		
299.	(0.00001)	RY*(10)	C	17	s( 0.82%)	p 8.09( 6.62%)	d99.99( 92.56%)		
300.	(0.00002)	RY*(11)	C	17	s( 73.77%)	p 0.32( 23.32%)	d 0.04( 2.92%)		
301.	(0.00000)	RY*(12)	C	17	s( 98.40%)	p 0.01( 0.86%)	d 0.01( 0.74%)		
302.	(0.00001)	RY*(13)	C	17	s( 9.67%)	p 2.36( 22.81%)	d 6.98( 67.52%)		
303.	(0.00001)	RY*(14)	C	17	s( 3.16%)	p 1.41( 4.47%)	d29.24( 92.37%)		
304.	(0.00206)	RY*( 1)	C	18	s( 0.57%)	p99.99( 69.17%)	d53.45( 30.26%)		
					0.0000	-0.0013	0.0711	-0.0245	0.0025
					-0.0054	-0.0071	-0.0092	0.0116	0.5858
					-0.1948	-0.0145	-0.5188	0.2025	-0.1383
					0.1114	0.0110	-0.2093	-0.4766	
305.	(0.00169)	RY*( 2)	C	18	s( 1.10%)	p78.90( 86.63%)	d11.18( 12.27%)		
					0.0000	0.0030	0.0790	0.0687	0.0027
					-0.0097	-0.8584	-0.2086	-0.0075	-0.2188
					0.0420	-0.0119	-0.1598	0.1019	-0.1755
					-0.1944	-0.1120	0.1688	-0.1146	
306.	(0.00084)	RY*( 3)	C	18	s( 31.75%)	p 2.13( 67.76%)	d 0.02( 0.49%)		
					0.0000	-0.0019	0.5510	0.1178	-0.0055
					0.0141	-0.1169	-0.0003	-0.0230	0.4309
					0.2807	-0.0216	0.5419	0.3233	0.0262
					0.0205	-0.0249	-0.0280	0.0491	
307.	(0.00018)	RY*( 4)	C	18	s( 24.75%)	p 2.46( 60.96%)	d 0.58( 14.29%)		
					0.0000	-0.0046	0.4665	-0.1657	0.0491
					-0.0100	0.2383	-0.5551	0.0036	-0.2143
					-0.4181	0.0019	-0.0833	0.1298	0.2264
					0.0754	-0.1592	0.2454	-0.0206	
308.	(0.00011)	RY*( 5)	C	18	s( 12.58%)	p 2.83( 35.56%)	d 4.12( 51.85%)		
					0.0000	0.0047	-0.1529	0.3197	-0.0147
					-0.0028	0.1660	-0.2455	0.0121	-0.3610
					0.2469	0.0082	0.2487	0.1199	-0.0851
					0.2403	-0.0942	-0.1910	-0.6389	
309.	(0.00007)	RY*( 6)	C	18	s( 6.27%)	p11.30( 70.90%)	d 3.64( 22.82%)		
310.	(0.00005)	RY*( 7)	C	18	s( 10.77%)	p 4.21( 45.29%)	d 4.08( 43.93%)		
311.	(0.00003)	RY*( 8)	C	18	s( 16.49%)	p 3.96( 65.35%)	d 1.10( 18.16%)		
312.	(0.00001)	RY*( 9)	C	18	s( 18.70%)	p 1.62( 30.32%)	d 2.73( 50.98%)		
313.	(0.00002)	RY*(10)	C	18	s( 3.27%)	p 2.81( 9.19%)	d26.74( 87.54%)		
314.	(0.00001)	RY*(11)	C	18	s( 1.33%)	p 5.68( 7.57%)	d68.29( 91.10%)		
315.	(0.00002)	RY*(12)	C	18	s( 13.95%)	p 1.88( 26.26%)	d 4.29( 59.79%)		
316.	(0.00001)	RY*(13)	C	18	s( 60.69%)	p 0.40( 24.04%)	d 0.25( 15.27%)		
317.	(0.00000)	RY*(14)	C	18	s( 97.70%)	p 0.01( 1.27%)	d 0.01( 1.03%)		
318.	(0.00033)	RY*( 1)	H	19	s( 96.37%)	p 0.04( 3.63%)			
					0.0005	0.9817	-0.0018	0.0053	0.1849
					-0.0458				
319.	(0.00027)	RY*( 2)	H	19	s( 0.04%)	p99.99( 99.96%)			
					0.0000	0.0180	-0.0053	0.0596	-0.3305
					-0.9417				
320.	(0.00017)	RY*( 3)	H	19	s( 78.75%)	p 0.27( 21.25%)			
					0.0019	0.0741	0.8843	0.2559	-0.3577
					0.1382				
321.	(0.00015)	RY*( 4)	H	19	s( 23.65%)	p 3.23( 76.35%)			
					-0.0007	-0.1497	0.4627	-0.3680	0.7384
					-0.2879				
322.	(0.00004)	RY*( 5)	H	19	s( 1.26%)	p78.22( 98.74%)			
323.	(0.00047)	RY*( 1)	H	20	s( 97.72%)	p 0.02( 2.28%)			
					-0.0003	0.9885	0.0056	-0.0864	-0.1132
					0.0503				
324.	(0.00028)	RY*( 2)	H	20	s( 0.04%)	p99.99( 99.96%)			
					0.0001	0.0142	-0.0132	0.0604	-0.3396
					-0.9384				
325.	(0.00020)	RY*( 3)	H	20	s( 99.33%)	p 0.01( 0.67%)			
					0.0014	-0.0077	0.9966	0.0579	-0.0573

326.	(0.00016)	RY*( 4)	H	20	0.0104 s( 1.90%)p51.63( 98.10%) 0.0014 0.1365 -0.0195 0.8553 0.4852 -0.1182
327.	(0.00004)	RY*( 5)	H	20	s( 1.08%)p91.58( 98.92%)
328.	(0.00036)	RY*( 1)	H	21	s( 98.22%)p 0.02( 1.78%) -0.0001 0.9910 0.0052 0.0268 0.0961 0.0886
329.	(0.00029)	RY*( 2)	H	21	s( 0.07%)p99.99( 99.93%) 0.0003 -0.0025 0.0267 0.0814 -0.6746 0.7332
330.	(0.00017)	RY*( 3)	H	21	s( 97.77%)p 0.02( 2.23%) 0.0006 -0.0246 0.9885 0.0523 0.1212 0.0696
331.	(0.00016)	RY*( 4)	H	21	s( 3.33%)p29.06( 96.67%) 0.0013 0.1153 0.1413 -0.6345 -0.5843 -0.4719
332.	(0.00004)	RY*( 5)	H	21	s( 0.67%)p99.99( 99.33%)
333.	(0.00034)	RY*( 1)	H	22	s( 94.32%)p 0.06( 5.68%) 0.0009 0.9712 -0.0025 0.0111 -0.0201 -0.2371
334.	(0.00030)	RY*( 2)	H	22	s( 2.30%)p42.55( 97.70%) -0.0008 0.1513 0.0082 0.1478 -0.6964 0.6857
335.	(0.00017)	RY*( 3)	H	22	s( 93.12%)p 0.07( 6.88%) 0.0004 0.0409 0.9641 -0.1902 0.1162 0.1384
336.	(0.00016)	RY*( 4)	H	22	s( 9.22%)p 9.85( 90.78%) -0.0015 -0.1477 0.2652 0.6616 -0.4212 -0.5410
337.	(0.00004)	RY*( 5)	H	22	s( 1.11%)p89.16( 98.89%)
338.	(0.00051)	RY*( 1)	H	23	s( 81.87%)p 0.22( 18.13%) -0.0022 0.9030 0.0575 -0.2460 -0.2866 -0.1965
339.	(0.00021)	RY*( 2)	H	23	s( 43.57%)p 1.30( 56.43%) -0.0060 -0.3659 0.5493 -0.2129 -0.5128 -0.5060
340.	(0.00014)	RY*( 3)	H	23	s( 2.83%)p34.39( 97.17%) 0.0013 0.1158 0.1218 0.2910 0.6236 -0.7059
341.	(0.00010)	RY*( 4)	H	23	s( 67.82%)p 0.47( 32.18%)
342.	(0.00002)	RY*( 5)	H	23	s( 3.97%)p24.18( 96.03%)
343.	(0.00139)	RY*( 1)	H	24	s( 90.54%)p 0.10( 9.46%) -0.0040 0.9515 0.0069 0.0073 -0.2867 -0.1111
344.	(0.00020)	RY*( 2)	H	24	s( 57.92%)p 0.73( 42.08%) -0.0006 -0.0848 0.7563 -0.5535 -0.3200 0.1100
345.	(0.00015)	RY*( 3)	H	24	s( 7.66%)p12.05( 92.34%) 0.0006 0.2747 -0.0341 -0.3701 0.6817 0.5672
346.	(0.00009)	RY*( 4)	H	24	s( 43.68%)p 1.29( 56.32%)
347.	(0.00003)	RY*( 5)	H	24	s( 0.24%)p99.99( 99.76%)
348.	(0.00187)	RY*( 1)	H	25	s( 94.98%)p 0.05( 5.02%) -0.0024 0.9746 0.0028 0.0684 -0.1890 -0.0989
349.	(0.00028)	RY*( 2)	H	25	s( 80.86%)p 0.24( 19.14%) -0.0003 -0.0499 0.8978 -0.2207 -0.1404 -0.3506
350.	(0.00016)	RY*( 3)	H	25	s( 11.75%)p 7.51( 88.25%) -0.0047 0.2128 0.2688 -0.2653 0.7255 0.5345
351.	(0.00010)	RY*( 4)	H	25	s( 12.07%)p 7.29( 87.93%) 0.0005 -0.0465 0.3443 0.6782 -0.2918 0.5781
352.	(0.00004)	RY*( 5)	H	25	s( 0.39%)p99.99( 99.61%)
353.	(0.00084)	RY*( 1)	H	26	s( 90.48%)p 0.11( 9.52%) -0.0028 0.9509 0.0257 -0.1743 0.1328 0.2171
354.	(0.00023)	RY*( 2)	H	26	s( 33.40%)p 1.99( 66.60%) -0.0046 -0.2703 0.5108 -0.4575 0.5087

355.	(0.00014)	RY*( 3)	H	26	0.4449 s( 17.75%)p 4.64( 82.25%) 0.0010 0.0244 0.4206 0.6480 -0.3106 0.5534
356.	(0.00009)	RY*( 4)	H	26	s( 56.77%)p 0.76( 43.23%)
357.	(0.00002)	RY*( 5)	H	26	s( 1.64%)p59.81( 98.36%)
358.	(0.00137)	RY*( 1)	H	27	s( 89.15%)p 0.12( 10.85%) -0.0041 0.9441 0.0113 -0.1266 0.2677 0.1444
359.	(0.00017)	RY*( 2)	H	27	s( 53.25%)p 0.88( 46.75%) 0.0000 -0.2004 0.7016 -0.5833 0.2871 0.2119
360.	(0.00014)	RY*( 3)	H	27	s( 8.16%)p11.25( 91.84%) 0.0010 -0.1063 0.2652 0.7192 0.6082 0.1770
361.	(0.00009)	RY*( 4)	H	27	s( 49.39%)p 1.02( 50.61%)
362.	(0.00003)	RY*( 5)	H	27	s( 0.10%)p99.99( 99.90%)
363.	(0.00079)	RY*( 1)	H	28	s( 98.23%)p 0.02( 1.77%) -0.0031 0.9911 -0.0081 -0.0190 0.1218 0.0500
364.	(0.00024)	RY*( 2)	H	28	s( 27.23%)p 2.67( 72.77%) -0.0045 0.1123 0.5095 -0.1561 -0.7956 -0.2654
365.	(0.00018)	RY*( 3)	H	28	s( 29.75%)p 2.36( 70.25%) -0.0012 -0.0540 0.5427 -0.2088 0.1128 0.8039
366.	(0.00008)	RY*( 4)	H	28	s( 39.11%)p 1.56( 60.89%)
367.	(0.00003)	RY*( 5)	H	28	s( 5.74%)p16.42( 94.26%)
368.	(0.00080)	RY*( 1)	H	29	s( 84.30%)p 0.19( 15.70%) -0.0036 0.9178 0.0260 0.2692 0.2896 -0.0261
369.	(0.00018)	RY*( 2)	H	29	s( 46.54%)p 1.15( 53.46%) -0.0019 -0.3325 0.5957 0.4887 0.5428 -0.0329
370.	(0.00015)	RY*( 3)	H	29	s( 11.72%)p 7.53( 88.28%) 0.0008 0.0956 0.3287 -0.8007 0.4328 0.2331
371.	(0.00009)	RY*( 4)	H	29	s( 57.22%)p 0.75( 42.78%)
372.	(0.00003)	RY*( 5)	H	29	s( 0.27%)p99.99( 99.73%)
373.	(0.00071)	RY*( 1)	H	30	s( 91.28%)p 0.10( 8.72%) -0.0018 0.9546 -0.0392 0.1456 0.2461 -0.0739
374.	(0.00028)	RY*( 2)	H	30	s( 51.49%)p 0.94( 48.51%) -0.0087 0.2101 0.6860 0.0209 -0.6281 0.3002
375.	(0.00011)	RY*( 3)	H	30	s( 46.14%)p 1.17( 53.86%) -0.0001 -0.1926 0.6514 0.3263 0.6574 -0.0009
376.	(0.00010)	RY*( 4)	H	30	s( 3.52%)p27.37( 96.48%) -0.0015 -0.0187 0.1868 0.1155 -0.2492 -0.9430
377.	(0.00003)	RY*( 5)	H	30	s( 7.62%)p12.12( 92.38%)
378.	(0.00090)	RY*( 1)	H	31	s( 85.35%)p 0.17( 14.65%) -0.0036 0.9235 0.0240 0.2572 0.2407 -0.1498
379.	(0.00018)	RY*( 2)	H	31	s( 51.35%)p 0.95( 48.65%) -0.0015 -0.3058 0.6480 0.4642 0.4340 -0.2875
380.	(0.00014)	RY*( 3)	H	31	s( 8.37%)p10.95( 91.63%) 0.0005 0.0884 0.2754 -0.8093 0.2071 -0.4674
381.	(0.00009)	RY*( 4)	H	31	s( 54.44%)p 0.84( 45.56%)
382.	(0.00003)	RY*( 5)	H	31	s( 0.54%)p99.99( 99.46%)
383.	(0.00067)	RY*( 1)	H	32	s( 79.36%)p 0.26( 20.64%) -0.0037 0.8899 0.0416 0.0707 -0.3911 0.2201
384.	(0.00019)	RY*( 2)	H	32	s( 56.74%)p 0.76( 43.26%) -0.0017 -0.3291 0.6775 -0.1791 -0.4714 0.4223
385.	(0.00015)	RY*( 3)	H	32	s( 3.56%)p27.13( 96.44%) 0.0001 0.1886 0.0013 -0.8985 0.3601

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                                0.1657
386. (0.00009) RY*( 4) H 32      s( 60.06%)p 0.66( 39.94%)
387. (0.00003) RY*( 5) H 32      s(  0.33%)p99.99( 99.67%)
388. (0.00074) RY*( 1) H 33      s( 80.13%)p 0.25( 19.87%)
                                -0.0038  0.8944  0.0355  0.0634 -0.4339
                                0.0803
389. (0.00018) RY*( 2) H 33      s( 58.35%)p 0.71( 41.65%)
                                -0.0015 -0.3145  0.6962 -0.1705 -0.6217
                                -0.0295
390. (0.00014) RY*( 3) H 33      s(  2.86%)p33.95( 97.14%)
                                -0.0002  0.1592 -0.0572 -0.8946  0.1195
                                -0.3960
391. (0.00009) RY*( 4) H 33      s( 58.45%)p 0.71( 41.55%)
392. (0.00003) RY*( 5) H 33      s(  0.25%)p99.99( 99.75%)
393. (0.00217) RY*( 1) H 34      s( 93.85%)p 0.07(  6.15%)
                                -0.0014  0.9687 -0.0137 -0.0789 -0.2263
                                0.0635
394. (0.00035) RY*( 2) H 34      s( 77.16%)p 0.30( 22.84%)
                                -0.0035  0.1327  0.8683  0.2158  0.4209
                                -0.0681
395. (0.00012) RY*( 3) H 34      s( 24.75%)p 3.04( 75.25%)
                                0.0079 -0.1942  0.4580 -0.4774 -0.5655
                                0.4525
396. (0.00010) RY*( 4) H 34      s(  3.66%)p26.34( 96.34%)
397. (0.00004) RY*( 5) H 34      s(  0.64%)p99.99( 99.36%)
398. (0.04797) BD*( 1) N   1 - C   2
      ( 37.59%)  0.6131* N   1 s( 34.50%)p 1.90( 65.45%)d 0.00(  0.06%)
                                0.0001 -0.5873 -0.0058  0.0055 -0.0001
                                0.3369 -0.0120 -0.0004 -0.6846 -0.0052
                                0.0072  0.2686  0.0014 -0.0024  0.0102
                                -0.0042  0.0135  0.0133  0.0098
      ( 62.41%) -0.7900* C   2 s( 26.95%)p 2.71( 72.97%)d 0.00(  0.07%)
                                0.0003 -0.5185 -0.0253 -0.0003 -0.0001
                                -0.2518  0.0114  0.0011  0.7624  0.0194
                                0.0172 -0.2903 -0.0065 -0.0062  0.0184
                                -0.0071  0.0123  0.0110  0.0093
399. (0.02785) BD*( 1) N   1 - C   5
      ( 38.27%)  0.6187* N   1 s( 32.56%)p 2.07( 67.39%)d 0.00(  0.05%)
                                0.0000 -0.5706  0.0027 -0.0014  0.0000
                                -0.8154  0.0015  0.0034  0.0606 -0.0166
                                0.0099 -0.0703  0.0060 -0.0033 -0.0033
                                -0.0013  0.0000 -0.0200  0.0116
      ( 61.73%) -0.7857* C   5 s( 28.77%)p 2.47( 71.15%)d 0.00(  0.08%)
                                0.0001 -0.5362 -0.0119  0.0034  0.0010
                                0.8370  0.0353 -0.0069  0.0916  0.0221
                                0.0122  0.0224 -0.0056 -0.0048  0.0028
                                -0.0044  0.0017 -0.0233  0.0155
400. (0.01663) BD*( 1) N   1 - C  10
      ( 37.39%)  0.6115* N   1 s( 32.89%)p 2.04( 67.08%)d 0.00(  0.02%)
                                0.0001 -0.5735  0.0077 -0.0034  0.0001
                                0.4666  0.0020 -0.0083  0.6411 -0.0001
                                -0.0020 -0.2048  0.0002  0.0004 -0.0126
                                0.0040  0.0051  0.0024  0.0066
      ( 62.61%) -0.7913* C  10 s( 24.82%)p 3.03( 75.10%)d 0.00(  0.08%)
                                -0.0001 -0.4975 -0.0259  0.0006  0.0002
                                -0.5328 -0.0212  0.0041 -0.6492 -0.0194
                                0.0050  0.2117  0.0063 -0.0016 -0.0219
                                0.0072  0.0091  0.0050  0.0114
401. (0.04502) BD*( 1) C   2 - N   3
      ( 62.35%)  0.7896* C   2 s( 26.62%)p 2.75( 73.30%)d 0.00(  0.07%)
                                0.0003 -0.5154 -0.0240 -0.0016 -0.0001
                                -0.6675 -0.0040 -0.0086 -0.5164 -0.0223
                                -0.0138  0.1415  0.0075  0.0042 -0.0193
                                0.0049  0.0025 -0.0130  0.0131
      ( 37.65%) -0.6136* N   3 s( 34.61%)p 1.89( 65.33%)d 0.00(  0.06%)
                                0.0001 -0.5883 -0.0057  0.0047 -0.0001
                                0.6902 -0.0070 -0.0039  0.4080  0.0117
                                -0.0060 -0.1012 -0.0043  0.0020 -0.0187
                                0.0047  0.0055 -0.0048  0.0127
402. (0.58815) BD*( 2) C   2 - N   3
      ( 73.24%)  0.8558* C   2 s(  0.00%)p 1.00( 99.85%)d 0.00(  0.15%)

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					0.0000	0.0030	0.0004	0.0003	0.0000
					-0.0648	-0.0029	0.0008	0.3377	0.0114
					-0.0036	0.9375	0.0328	-0.0101	0.0118
					0.0347	0.0113	-0.0068	-0.0037	
	( 26.76%)	-0.5173*	N	3	s( 0.00%)	p 1.00( 99.98%)	d 0.00( 0.02%)		
					0.0000	0.0017	0.0000	-0.0002	0.0000
					-0.0624	0.0000	-0.0005	0.3408	-0.0002
					0.0031	0.9379	-0.0006	0.0085	-0.0014
					-0.0063	-0.0102	0.0046	0.0065	
403.	(0.05872)	BD*( 1)	C	2 - B	6				
	( 34.42%)	0.5866*	C	2	s( 46.47%)	p 1.15( 53.53%)	d 0.00( 0.00%)		
					0.0000	0.6815	-0.0174	-0.0024	0.0000
					-0.6960	0.0350	0.0114	0.1881	-0.0105
					-0.0033	-0.1179	0.0043	0.0030	-0.0024
					0.0023	-0.0016	0.0038	-0.0039	
	( 65.58%)	-0.8098*	B	6	s( 36.56%)	p 1.73( 63.40%)	d 0.00( 0.04%)		
					-0.0011	0.6046	0.0014	-0.0031	0.0022
					0.7492	0.0073	0.0129	-0.2380	-0.0031
					-0.0041	0.1257	0.0028	0.0026	-0.0083
					0.0050	-0.0020	0.0145	-0.0110	
404.	(0.02694)	BD*( 1)	N	3 - C	4				
	( 38.40%)	0.6197*	N	3	s( 32.32%)	p 2.09( 67.62%)	d 0.00( 0.06%)		
					0.0000	-0.5685	0.0034	-0.0008	0.0000
					-0.7202	0.0118	-0.0028	0.3551	0.0133
					-0.0101	-0.1759	-0.0041	0.0034	0.0181
					-0.0080	0.0060	-0.0059	0.0096	
	( 61.60%)	-0.7848*	C	4	s( 28.88%)	p 2.46( 71.03%)	d 0.00( 0.08%)		
					0.0001	-0.5373	-0.0119	0.0033	0.0010
					0.6505	0.0162	-0.0129	-0.4883	-0.0359
					-0.0068	0.2164	0.0138	0.0014	0.0177
					-0.0090	0.0060	-0.0137	0.0140	
405.	(0.01793)	BD*( 1)	N	3 - C	9				
	( 36.96%)	0.6079*	N	3	s( 33.01%)	p 2.03( 66.97%)	d 0.00( 0.02%)		
					0.0001	-0.5745	0.0066	-0.0033	0.0001
					0.0059	0.0007	-0.0051	-0.7686	-0.0021
					0.0056	0.2807	0.0008	-0.0024	0.0013
					-0.0005	0.0087	0.0114	0.0050	
	( 63.04%)	-0.7940*	C	9	s( 24.53%)	p 3.07( 75.40%)	d 0.00( 0.08%)		
					-0.0001	-0.4945	-0.0269	0.0013	0.0002
					-0.0376	-0.0061	0.0014	0.8133	0.0289
					-0.0069	-0.3002	-0.0110	0.0024	0.0020
					-0.0007	0.0155	0.0210	0.0088	
406.	(0.00852)	BD*( 1)	C	4 - C	5				
	( 50.04%)	0.7074*	C	4	s( 37.00%)	p 1.70( 62.93%)	d 0.00( 0.06%)		
					0.0001	-0.6083	-0.0065	-0.0006	-0.0001
					0.1378	-0.0167	-0.0206	0.7380	0.0273
					-0.0041	-0.2532	-0.0109	0.0002	-0.0155
					0.0047	0.0112	0.0108	0.0114	
	( 49.96%)	-0.7069*	C	5	s( 37.07%)	p 1.70( 62.87%)	d 0.00( 0.06%)		
					0.0001	-0.6088	-0.0062	-0.0007	-0.0001
					-0.3192	-0.0301	-0.0151	-0.6882	-0.0153
					0.0137	0.2272	0.0034	-0.0058	-0.0052
					0.0015	0.0141	0.0173	0.0104	
407.	(0.29507)	BD*( 2)	C	4 - C	5				
	( 50.20%)	0.7085*	C	4	s( 0.00%)	p 1.00( 99.96%)	d 0.00( 0.04%)		
					0.0000	0.0005	0.0005	-0.0001	0.0000
					-0.0612	0.0022	-0.0011	0.3341	-0.0125
					0.0060	0.9394	-0.0352	0.0168	-0.0028
					-0.0109	-0.0128	0.0059	0.0078	
	( 49.80%)	-0.7057*	C	5	s( 0.00%)	p 1.00( 99.96%)	d 0.00( 0.04%)		
					0.0000	0.0011	0.0004	0.0000	0.0000
					-0.0613	0.0023	-0.0011	0.3372	-0.0127
					0.0060	0.9383	-0.0357	0.0169	-0.0013
					0.0000	0.0150	-0.0061	-0.0108	
408.	(0.01201)	BD*( 1)	C	4 - H	19				
	( 38.31%)	0.6190*	C	4	s( 34.06%)	p 1.94( 65.92%)	d 0.00( 0.02%)		
					0.0003	-0.5835	0.0105	-0.0013	-0.0006
					-0.7432	0.0076	0.0056	-0.3198	0.0086
					0.0075	0.0656	-0.0026	-0.0023	-0.0102
					0.0024	0.0001	-0.0078	0.0058	
	( 61.69%)	-0.7854*	H	19	s( 99.94%)	p 0.00( 0.06%)			



-0.9997 -0.0015 -0.0002 0.0229 0.0095  
 -0.0019  
 409. (0.01274) BD\*( 1) C 5 - H 20  
 ( 38.37%) 0.6194\* C 5 s( 34.12%)p 1.93( 65.86%)d 0.00( 0.02%)  
 -0.0003 0.5840 -0.0103 0.0014 0.0006  
 0.4361 -0.0005 -0.0005 -0.6346 0.0109  
 0.0091 0.2559 -0.0039 -0.0033 -0.0105  
 0.0040 -0.0058 -0.0055 -0.0037  
 ( 61.63%) -0.7851\* H 20 s( 99.94%)p 0.00( 0.06%)  
 0.9997 0.0017 0.0006 -0.0139 0.0192  
 -0.0078  
 410. (0.07253) BD\*( 1) B 6 - C 7  
 ( 59.82%) 0.7734\* B 6 s( 28.33%)p 2.53( 71.61%)d 0.00( 0.06%)  
 -0.0009 0.5323 -0.0027 0.0037 -0.0007  
 -0.1303 0.0092 -0.0041 0.7668 0.0056  
 0.0098 -0.3330 -0.0004 -0.0053 -0.0139  
 0.0060 -0.0092 -0.0087 -0.0141  
 ( 40.18%) -0.6339\* C 7 s( 39.27%)p 1.55( 60.71%)d 0.00( 0.02%)  
 -0.0002 0.6254 -0.0385 0.0021 -0.0004  
 0.6986 0.0031 -0.0002 -0.3441 -0.0064  
 0.0066 0.0222 -0.0012 -0.0024 -0.0125  
 0.0040 -0.0029 -0.0026 -0.0065  
 411. (0.03873) BD\*( 1) B 6 - B 11  
 ( 50.09%) 0.7077\* B 6 s( 34.70%)p 1.88( 65.28%)d 0.00( 0.03%)  
 -0.0005 -0.5890 -0.0067 0.0007 0.0009  
 0.6430 -0.0077 -0.0119 0.4816 -0.0043  
 0.0048 -0.0839 -0.0015 -0.0012 0.0000  
 0.0010 0.0022 -0.0143 0.0064  
 ( 49.91%) -0.7065\* B 11 s( 40.21%)p 1.49( 59.76%)d 0.00( 0.02%)  
 -0.0001 -0.6341 0.0031 -0.0001 0.0006  
 -0.6572 -0.0120 0.0145 0.4042 -0.0202  
 0.0056 -0.0380 0.0075 -0.0049 -0.0067  
 0.0049 -0.0006 -0.0112 0.0051  
 412. (0.04637) BD\*( 1) C 7 - O 8  
 ( 64.27%) 0.8017\* C 7 s( 33.83%)p 1.95( 66.08%)d 0.00( 0.09%)  
 -0.0003 0.5766 0.0766 0.0013 0.0010  
 -0.1172 0.0090 -0.0016 0.7975 -0.0521  
 0.0063 -0.0894 0.0159 0.0007 -0.0083  
 0.0009 -0.0059 -0.0251 -0.0134  
 ( 35.73%) -0.5978\* O 8 s( 38.87%)p 1.57( 61.00%)d 0.00( 0.13%)  
 0.0000 0.6232 -0.0183 0.0046 0.0001  
 0.1123 -0.0038 -0.0007 -0.7057 0.0322  
 -0.0020 0.3132 -0.0101 -0.0007 -0.0087  
 0.0032 -0.0179 -0.0275 -0.0117  
 413. (0.43205) BD\*( 2) C 7 - O 8  
 ( 71.79%) 0.8473\* C 7 s( 0.61%)p99.99( 99.15%)d 0.39( 0.24%)  
 0.0002 -0.0764 -0.0157 0.0039 0.0002  
 0.1280 -0.0021 -0.0009 0.1848 0.0124  
 0.0030 0.9698 -0.0008 0.0184 0.0041  
 -0.0102 0.0424 -0.0111 -0.0181  
 ( 28.21%) -0.5311\* O 8 s( 0.47%)p99.99( 99.43%)d 0.21( 0.10%)  
 0.0000 -0.0682 0.0041 0.0001 -0.0001  
 0.1246 -0.0031 -0.0006 0.3669 -0.0092  
 0.0000 0.9187 -0.0127 -0.0021 -0.0016  
 0.0051 -0.0243 0.0123 0.0149  
 414. (0.11509) BD\*( 1) C 7 - B 11  
 ( 40.81%) 0.6388\* C 7 s( 26.79%)p 2.73( 73.18%)d 0.00( 0.03%)  
 0.0001 0.5172 -0.0213 -0.0033 -0.0001  
 -0.6932 -0.0041 0.0008 -0.4508 -0.0179  
 0.0065 0.2180 0.0102 -0.0006 0.0120  
 -0.0049 -0.0065 -0.0048 -0.0070  
 ( 59.19%) -0.7693\* B 11 s( 20.12%)p 3.97( 79.83%)d 0.00( 0.05%)  
 -0.0038 0.4483 -0.0134 0.0038 -0.0044  
 0.0996 -0.0058 -0.0066 0.8375 -0.0007  
 0.0084 -0.2944 0.0018 -0.0122 0.0082  
 0.0000 -0.0101 -0.0095 -0.0166  
 415. (0.01137) BD\*( 1) C 9 - H 32  
 ( 39.32%) 0.6271\* C 9 s( 24.29%)p 3.12( 75.67%)d 0.00( 0.04%)  
 0.0001 -0.4928 0.0065 -0.0019 -0.0002  
 -0.3921 0.0096 -0.0009 -0.5272 -0.0065  
 -0.0061 -0.5699 0.0066 -0.0011 -0.0090

-0.0117 -0.0131 0.0010 -0.0053  
 ( 60.68%) -0.7790\* H 32 s( 99.95%)p 0.00( 0.05%)  
 -0.9998 -0.0020 -0.0002 0.0078 0.0144  
 0.0142  
 416. (0.01225) BD\*( 1) C 9 - H 33  
 ( 39.31%) 0.6269\* C 9 s( 24.33%)p 3.11( 75.63%)d 0.00( 0.04%)  
 0.0001 -0.4932 0.0065 -0.0019 -0.0001  
 -0.4265 0.0101 -0.0016 -0.0395 -0.0090  
 -0.0040 0.7567 -0.0001 0.0045 0.0005  
 0.0156 -0.0016 -0.0045 -0.0124  
 ( 60.69%) -0.7791\* H 33 s( 99.95%)p 0.00( 0.05%)  
 -0.9998 -0.0022 -0.0002 0.0088 0.0018  
 -0.0197  
 417. (0.00878) BD\*( 1) C 9 - H 34  
 ( 35.52%) 0.5960\* C 9 s( 26.91%)p 2.71( 73.04%)d 0.00( 0.04%)  
 -0.0001 0.5187 -0.0035 -0.0026 -0.0001  
 -0.8137 0.0120 0.0068 0.2375 0.0028  
 0.0079 -0.1082 -0.0009 -0.0024 -0.0058  
 0.0029 0.0007 0.0176 -0.0092  
 ( 64.48%) -0.8030\* H 34 s( 99.94%)p 0.00( 0.06%)  
 0.9997 0.0021 0.0003 0.0240 -0.0049  
 0.0025  
 418. (0.01206) BD\*( 1) C 10 - H 29  
 ( 39.26%) 0.6266\* C 10 s( 24.52%)p 3.08( 75.44%)d 0.00( 0.04%)  
 0.0001 -0.4951 0.0079 -0.0020 -0.0001  
 -0.1481 0.0110 0.0034 0.2313 0.0025  
 0.0033 -0.8239 0.0061 -0.0053 0.0017  
 -0.0078 0.0069 -0.0003 -0.0176  
 ( 60.74%) -0.7794\* H 29 s( 99.95%)p 0.00( 0.05%)  
 -0.9998 -0.0023 -0.0002 0.0019 -0.0051  
 0.0208  
 419. (0.01214) BD\*( 1) C 10 - H 30  
 ( 36.22%) 0.6018\* C 10 s( 26.23%)p 2.81( 73.73%)d 0.00( 0.04%)  
 -0.0001 0.5122 -0.0007 -0.0036 0.0000  
 -0.8167 0.0038 0.0028 0.2486 -0.0085  
 -0.0090 -0.0910 0.0035 0.0032 -0.0135  
 0.0046 -0.0017 0.0116 -0.0090  
 ( 63.78%) -0.7987\* H 30 s( 99.95%)p 0.00( 0.05%)  
 0.9997 0.0018 0.0009 0.0197 -0.0099  
 0.0035  
 420. (0.01312) BD\*( 1) C 10 - H 31  
 ( 39.32%) 0.6271\* C 10 s( 24.49%)p 3.08( 75.47%)d 0.00( 0.04%)  
 -0.0001 0.4948 -0.0080 0.0023 0.0001  
 0.1611 -0.0106 -0.0028 -0.6791 0.0016  
 -0.0061 -0.5170 0.0059 -0.0022 -0.0066  
 -0.0053 0.0165 -0.0087 0.0022  
 ( 60.68%) -0.7789\* H 31 s( 99.95%)p 0.00( 0.05%)  
 0.9998 0.0025 0.0002 -0.0026 0.0166  
 0.0135  
 421. (0.03334) BD\*( 1) B 11 - C 12  
 ( 66.12%) 0.8132\* B 11 s( 39.46%)p 1.53( 60.49%)d 0.00( 0.05%)  
 -0.0003 0.6281 0.0102 0.0017 0.0042  
 -0.7398 -0.0165 -0.0138 -0.2056 -0.0036  
 -0.0051 0.1214 0.0024 0.0037 0.0073  
 -0.0053 -0.0003 0.0182 -0.0114  
 ( 33.88%) -0.5820\* C 12 s( 46.47%)p 1.15( 53.52%)d 0.00( 0.01%)  
 -0.0001 0.6815 -0.0161 -0.0066 0.0000  
 0.7231 -0.0379 -0.0074 0.0878 -0.0059  
 -0.0017 -0.0551 0.0012 0.0018 0.0033  
 -0.0028 0.0032 0.0061 -0.0035  
 422. (0.04275) BD\*( 1) C 12 - N 13  
 ( 61.95%) 0.7871\* C 12 s( 26.73%)p 2.74( 73.20%)d 0.00( 0.07%)  
 -0.0003 0.5165 0.0208 0.0058 0.0000  
 -0.5084 -0.0003 -0.0015 0.4869 0.0186  
 0.0113 0.4854 0.0159 0.0101 -0.0160  
 -0.0159 0.0125 0.0070 -0.0045  
 ( 38.05%) -0.6169\* N 13 s( 33.66%)p 1.97( 66.28%)d 0.00( 0.06%)  
 -0.0001 0.5801 0.0063 -0.0066 0.0001  
 0.5611 -0.0101 -0.0040 -0.4027 -0.0046  
 0.0071 -0.4308 -0.0053 0.0061 -0.0129  
 -0.0132 0.0154 0.0019 -0.0019

423. (0.69287) BD\*( 2) C 12 - N 13  
( 74.35%) 0.8622\* C 12 s( 0.00%)p 1.00( 99.85%)d 0.00( 0.15%)  
0.0002 0.0054 0.0016 -0.0014 0.0002  
0.1298 0.0100 -0.0060 -0.6309 -0.0207  
0.0037 0.7632 0.0244 -0.0060 0.0221  
-0.0215 0.0008 0.0040 0.0222  
( 25.65%) -0.5065\* N 13 s( 0.00%)p 1.00( 99.98%)d 0.00( 0.02%)  
0.0000 0.0002 0.0003 -0.0006 0.0000  
0.1266 0.0000 0.0013 -0.6367 -0.0008  
-0.0058 0.7605 0.0015 0.0076 -0.0031  
0.0008 -0.0024 -0.0054 -0.0111

424. (0.04534) BD\*( 1) C 12 - N 16  
( 62.03%) 0.7876\* C 12 s( 26.81%)p 2.73( 73.12%)d 0.00( 0.07%)  
-0.0003 0.5173 0.0219 0.0066 0.0000  
-0.4467 0.0046 0.0000 -0.5953 -0.0188  
-0.0125 -0.4200 -0.0148 -0.0098 0.0190  
0.0123 0.0133 0.0021 -0.0057  
( 37.97%) -0.6162\* N 16 s( 34.05%)p 1.93( 65.89%)d 0.00( 0.06%)  
-0.0001 0.5835 0.0069 -0.0062 0.0001  
0.5204 -0.0104 -0.0035 0.4826 0.0041  
-0.0078 0.3936 0.0047 -0.0059 0.0147  
0.0090 0.0157 -0.0021 -0.0041

425. (0.02556) BD\*( 1) N 13 - C 14  
( 38.32%) 0.6190\* N 13 s( 33.09%)p 2.02( 66.86%)d 0.00( 0.05%)  
0.0000 -0.5752 0.0018 -0.0024 0.0000  
0.7870 -0.0084 0.0006 0.2153 0.0120  
-0.0088 0.0494 0.0103 -0.0075 -0.0135  
-0.0060 -0.0029 -0.0138 0.0108  
( 61.68%) -0.7854\* C 14 s( 28.77%)p 2.47( 71.16%)d 0.00( 0.08%)  
0.0001 -0.5362 -0.0110 0.0027 0.0012  
-0.7622 -0.0259 0.0105 -0.3142 -0.0267  
-0.0075 -0.1729 -0.0196 -0.0076 -0.0113  
-0.0037 -0.0033 -0.0211 0.0138

426. (0.01595) BD\*( 1) N 13 - C 17  
( 37.57%) 0.6130\* N 13 s( 33.19%)p 2.01( 66.78%)d 0.00( 0.03%)  
0.0001 -0.5761 0.0086 -0.0034 0.0001  
-0.2210 -0.0029 0.0073 -0.6210 0.0012  
0.0036 -0.4830 0.0016 0.0017 -0.0068  
-0.0053 -0.0124 0.0057 0.0002  
( 62.43%) -0.7901\* C 17 s( 25.24%)p 2.96( 74.68%)d 0.00( 0.08%)  
-0.0001 -0.5017 -0.0265 0.0018 0.0002  
0.2565 0.0124 -0.0008 0.6701 0.0221  
-0.0059 0.4807 0.0142 -0.0034 -0.0108  
-0.0081 -0.0206 0.0124 0.0013

427. (0.00849) BD\*( 1) C 14 - C 15  
( 49.99%) 0.7070\* C 14 s( 37.28%)p 1.68( 62.65%)d 0.00( 0.06%)  
-0.0001 0.6106 0.0066 0.0007 0.0002  
-0.0647 -0.0234 -0.0183 -0.5996 -0.0203  
0.0056 -0.5111 -0.0148 0.0073 -0.0052  
-0.0055 0.0222 -0.0090 0.0028  
( 50.01%) -0.7072\* C 15 s( 37.32%)p 1.68( 62.62%)d 0.00( 0.06%)  
-0.0001 0.6109 0.0068 0.0009 0.0002  
-0.1179 -0.0243 -0.0185 0.5701 0.0177  
-0.0084 0.5344 0.0181 -0.0052 0.0040  
0.0031 0.0225 -0.0099 0.0024

428. (0.30224) BD\*( 2) C 14 - C 15  
( 50.57%) 0.7111\* C 14 s( 0.00%)p 1.00( 99.96%)d 0.00( 0.04%)  
0.0001 -0.0061 -0.0024 0.0005 0.0000  
0.1047 -0.0040 0.0018 -0.6546 0.0253  
-0.0113 0.7473 -0.0275 0.0128 -0.0048  
0.0029 -0.0017 -0.0081 -0.0168  
( 49.43%) -0.7031\* C 15 s( 0.00%)p 1.00( 99.96%)d 0.00( 0.04%)  
-0.0001 -0.0047 0.0000 0.0000 0.0000  
0.0960 -0.0030 0.0017 -0.6666 0.0266  
-0.0116 0.7377 -0.0293 0.0116 -0.0013  
0.0045 0.0021 0.0099 0.0155

429. (0.01215) BD\*( 1) C 14 - H 21  
( 38.54%) 0.6208\* C 14 s( 33.90%)p 1.95( 66.08%)d 0.00( 0.02%)  
-0.0003 0.5821 -0.0101 0.0007 0.0007  
-0.6336 0.0044 0.0036 0.3330 -0.0072  
-0.0063 0.3851 -0.0075 -0.0057 -0.0092

-0.0098 0.0040 0.0042 -0.0012  
 ( 61.46%) -0.7839\* H 21 s( 99.94%)p 0.00( 0.06%)  
 0.9997 0.0016 0.0003 0.0200 -0.0097  
 -0.0116

430. (0.02647) BD\*( 1) C 15 - N 16  
 ( 61.73%) 0.7857\* C 15 s( 28.57%)p 2.50( 71.35%)d 0.00( 0.08%)  
 -0.0001 0.5344 0.0113 -0.0031 -0.0011  
 0.7864 0.0298 -0.0094 -0.1705 -0.0216  
 -0.0099 -0.2529 -0.0214 -0.0066 -0.0029  
 -0.0086 0.0030 0.0232 -0.0129  
 ( 38.27%) -0.6186\* N 16 s( 32.78%)p 2.05( 67.17%)d 0.00( 0.05%)  
 0.0000 0.5725 -0.0007 0.0023 0.0000  
 -0.8040 0.0076 0.0005 0.0538 0.0115  
 -0.0085 0.1484 0.0097 -0.0079 -0.0073  
 -0.0094 0.0027 0.0170 -0.0094

431. (0.01206) BD\*( 1) C 15 - H 22  
 ( 38.56%) 0.6210\* C 15 s( 34.05%)p 1.94( 65.93%)d 0.00( 0.02%)  
 0.0003 -0.5835 0.0104 -0.0008 -0.0006  
 0.5964 -0.0022 -0.0033 0.4467 -0.0077  
 -0.0070 0.3223 -0.0059 -0.0064 -0.0106  
 -0.0079 -0.0048 -0.0017 0.0030  
 ( 61.44%) -0.7838\* H 22 s( 99.94%)p 0.00( 0.06%)  
 -0.9997 -0.0016 -0.0002 -0.0189 -0.0130  
 -0.0100

432. (0.01628) BD\*( 1) N 16 - C 18  
 ( 37.96%) 0.6161\* N 16 s( 33.11%)p 2.02( 66.86%)d 0.00( 0.03%)  
 0.0001 -0.5754 0.0098 -0.0031 0.0001  
 -0.2725 -0.0013 0.0074 0.5435 -0.0018  
 -0.0018 0.5466 -0.0023 -0.0035 0.0061  
 0.0076 -0.0127 0.0027 -0.0040  
 ( 62.04%) -0.7877\* C 18 s( 25.65%)p 2.90( 74.28%)d 0.00( 0.08%)  
 -0.0001 -0.5058 -0.0261 0.0000 0.0002  
 0.3175 0.0135 -0.0015 -0.5550 -0.0159  
 0.0039 -0.5772 -0.0192 0.0026 0.0107  
 0.0114 -0.0210 0.0066 -0.0052

433. (0.00663) BD\*( 1) C 17 - H 23  
 ( 39.43%) 0.6279\* C 17 s( 24.24%)p 3.12( 75.72%)d 0.00( 0.04%)  
 0.0001 -0.4923 0.0047 -0.0026 -0.0003  
 0.6870 -0.0103 -0.0034 -0.5038 -0.0053  
 -0.0053 -0.1769 -0.0015 -0.0028 0.0148  
 0.0041 -0.0029 -0.0085 0.0095  
 ( 60.57%) -0.7783\* H 23 s( 99.95%)p 0.00( 0.05%)  
 -0.9997 -0.0013 -0.0002 -0.0166 0.0150  
 0.0043

434. (0.01955) BD\*( 1) C 17 - H 24  
 ( 39.25%) 0.6265\* C 17 s( 24.62%)p 3.06( 75.34%)d 0.00( 0.04%)  
 0.0001 -0.4962 0.0058 -0.0008 0.0001  
 -0.3335 -0.0059 0.0038 0.2921 -0.0094  
 -0.0018 -0.7460 0.0047 -0.0078 0.0070  
 -0.0104 0.0114 -0.0003 -0.0117  
 ( 60.75%) -0.7794\* H 24 s( 99.96%)p 0.00( 0.04%)  
 -0.9998 -0.0043 -0.0002 0.0090 -0.0071  
 0.0175

435. (0.01126) BD\*( 1) C 17 - H 25  
 ( 36.67%) 0.6056\* C 17 s( 25.95%)p 2.85( 74.01%)d 0.00( 0.05%)  
 0.0001 -0.5093 0.0061 0.0020 0.0001  
 -0.5918 0.0041 0.0068 -0.4582 0.0033  
 -0.0104 0.4238 -0.0109 -0.0024 -0.0098  
 0.0149 0.0107 -0.0043 0.0020  
 ( 63.33%) -0.7958\* H 25 s( 99.94%)p 0.00( 0.06%)  
 -0.9997 -0.0030 0.0000 0.0167 0.0106  
 -0.0136

436. (0.01138) BD\*( 1) C 18 - H 26  
 ( 39.45%) 0.6281\* C 18 s( 24.44%)p 3.09( 75.52%)d 0.00( 0.04%)  
 -0.0001 0.4943 -0.0072 0.0030 0.0003  
 -0.4176 0.0090 0.0040 -0.7589 0.0017  
 -0.0054 0.0680 -0.0063 -0.0016 0.0152  
 -0.0026 -0.0045 -0.0072 -0.0100  
 ( 60.55%) -0.7782\* H 26 s( 99.95%)p 0.00( 0.05%)  
 0.9997 0.0023 0.0003 0.0094 0.0201  
 -0.0019

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437. (0.01881) BD*( 1) C 18 - H 27
      ( 39.04%) 0.6248* C 18 s( 24.84%)p 3.02( 75.12%)d 0.00( 0.04%)
          -0.0001 0.4983 -0.0079 0.0012 -0.0002
          -0.1120 0.0097 -0.0015 0.3145 -0.0080
          -0.0013 -0.7997 0.0051 -0.0072 -0.0010
          0.0047 -0.0132 -0.0022 0.0147
      ( 60.96%) -0.7808* H 27 s( 99.96%)p 0.00( 0.04%)
          0.9998 0.0041 0.0003 0.0016 -0.0085
          0.0188

438. (0.01221) BD*( 1) C 18 - H 28
      ( 37.63%) 0.6134* C 18 s( 25.14%)p 2.98( 74.82%)d 0.00( 0.04%)
          0.0001 -0.5013 0.0018 0.0040 0.0000
          -0.8434 0.0038 0.0055 0.1246 0.0002
          0.0091 -0.1451 0.0099 0.0029 0.0016
          -0.0090 0.0014 -0.0159 0.0098
      ( 62.37%) -0.7898* H 28 s( 99.95%)p 0.00( 0.05%)
          -0.9998 -0.0029 -0.0002 0.0216 -0.0005
          0.0041

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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	Dev	Theta	Phi	Dev	Theta	Phi	Dev
1. BD ( 1) N 1 - C 2	109.7	112.0		109.5	115.4	3.2	70.0	286.7	5.1
2. BD ( 1) N 1 - C 5	86.8	1.2		85.2	356.2	5.2	90.8	188.3	7.5
3. BD ( 1) N 1 - C 10	75.6	232.3		75.5	234.2	1.8	104.1	50.4	1.9
4. BD ( 1) C 2 - N 3	98.5	34.6		99.9	39.1	4.7	82.6	211.3	3.4
5. BD ( 2) C 2 - N 3	98.5	34.6		20.1	100.9	90.1	20.3	100.4	90.1
6. BD ( 1) C 2 - B 6	99.8	163.9		99.3	165.0	1.2	80.8	342.3	1.7
7. BD ( 1) N 3 - C 4	76.3	328.3		77.5	333.3	5.0	105.4	140.9	7.3
8. BD ( 1) N 3 - C 9	110.2	91.5		110.0	90.1	1.3	69.7	272.9	1.3
9. BD ( 1) C 4 - C 5	72.2	252.3		71.0	262.5	9.8	106.1	62.2	9.8
10. BD ( 2) C 4 - C 5	72.2	252.3		19.9	100.4	89.9	20.1	100.3	89.9
13. BD ( 1) B 6 - C 7	103.2	123.9		113.2	99.1	25.5	88.6	333.9	31.9
14. BD ( 1) B 6 - B 11	85.8	184.9		83.7	217.7	32.7	87.3	329.2	36.3
15. BD ( 1) C 7 - O 8	104.7	98.9		95.5	98.3	9.2	66.1	279.1	9.2
16. BD ( 2) C 7 - O 8	104.7	98.9		166.6	238.0	85.6	157.3	251.3	84.4
17. BD ( 1) C 7 - B 11	73.5	240.6		74.8	213.6	26.0	109.7	84.1	22.5
20. BD ( 1) C 9 - H 34	97.0	164.4		97.6	162.7	1.9	--	--	--
22. BD ( 1) C 10 - H 30	96.5	161.5		95.7	164.1	2.7	--	--	--
24. BD ( 1) B 11 - C 12	83.0	191.1		80.9	195.6	4.9	94.4	6.7	5.1
25. BD ( 1) C 12 - N 13	56.7	140.0		54.8	134.6	4.8	122.4	323.8	3.3
26. BD ( 2) C 12 - N 13	56.7	140.0		40.2	281.7	90.3	139.6	101.2	90.3
27. BD ( 1) C 12 - N 16	118.8	228.6		120.1	234.8	5.6	60.6	43.4	4.6
28. BD ( 1) N 13 - C 14	97.9	199.0		93.7	195.7	5.3	76.8	24.1	7.3
29. BD ( 1) N 13 - C 17	55.0	69.1		53.7	70.6	1.8	123.7	248.7	1.3
30. BD ( 1) C 14 - C 15	131.7	272.6		129.8	260.2	9.6	47.7	105.5	9.6
31. BD ( 2) C 14 - C 15	131.7	272.6		138.5	99.1	89.6	137.6	98.3	89.4
33. BD ( 1) C 15 - N 16	103.8	351.8		108.7	345.9	7.4	79.3	175.9	5.1
35. BD ( 1) N 16 - C 18	132.9	298.5		131.9	296.3	1.9	47.8	120.2	1.4
36. BD ( 1) C 17 - H 23	78.7	143.6		77.9	142.6	1.2	--	--	--
38. BD ( 1) C 17 - H 25	119.9	37.4		118.9	38.7	1.5	--	--	--
41. BD ( 1) C 18 - H 28	80.1	352.7		81.1	350.9	2.1	--	--	--
60. LP ( 1) N 1	--	--		159.8	279.3	--	--	--	--
61. LP ( 1) B 6	--	--		21.3	104.1	--	--	--	--
62. LP ( 1) O 8	--	--		104.3	105.0	--	--	--	--
63. LP ( 2) O 8	--	--		100.4	7.8	--	--	--	--
64. LP*( 1) B 11	--	--		18.4	69.8	--	--	--	--
65. LP ( 1) N 16	--	--		43.6	277.2	--	--	--	--
402. BD*( 2) C 2 - N 3	98.5	34.6		20.1	100.9	90.1	20.3	100.4	90.1
407. BD*( 2) C 4 - C 5	72.2	252.3		19.9	100.4	89.9	20.1	100.3	89.9
413. BD*( 2) C 7 - O 8	104.7	98.9		166.6	238.0	85.6	157.3	251.3	84.4
414. BD*( 1) C 7 - B 11	73.5	240.6		74.8	213.6	26.0	109.7	84.1	22.5
423. BD*( 2) C 12 - N 13	56.7	140.0		40.2	281.7	90.3	139.6	101.2	90.3

428. BD\*( 2) C 14 - C 15 131.7 272.6 138.5 99.1 89.6 137.6 98.3 89.4

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

F(i,j)	Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.
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	within unit 1			
0.031	1. BD ( 1) N 1 - C 2	/123. RY*( 2) C 5	0.54	2.16
0.029	1. BD ( 1) N 1 - C 2	/124. RY*( 3) C 5	0.54	2.00
0.029	1. BD ( 1) N 1 - C 2	/193. RY*( 2) C 10	0.68	1.58
0.030	1. BD ( 1) N 1 - C 2	/399. BD*( 1) N 1 - C 5	1.01	1.09
0.021	1. BD ( 1) N 1 - C 2	/400. BD*( 1) N 1 - C 10	0.54	1.00
0.040	1. BD ( 1) N 1 - C 2	/403. BD*( 1) C 2 - B 6	1.66	1.17
0.060	1. BD ( 1) N 1 - C 2	/405. BD*( 1) N 3 - C 9	4.57	1.00
0.046	1. BD ( 1) N 1 - C 2	/409. BD*( 1) C 5 - H 20	2.56	1.05
0.025	1. BD ( 1) N 1 - C 2	/410. BD*( 1) B 6 - C 7	0.62	1.21
0.042	2. BD ( 1) N 1 - C 5	/ 80. RY*( 1) C 2	0.86	2.55
0.042	2. BD ( 1) N 1 - C 5	/ 83. RY*( 4) C 2	1.10	1.99
0.032	2. BD ( 1) N 1 - C 5	/194. RY*( 3) C 10	0.64	2.00
0.028	2. BD ( 1) N 1 - C 5	/398. BD*( 1) N 1 - C 2	0.85	1.11
0.025	2. BD ( 1) N 1 - C 5	/401. BD*( 1) C 2 - N 3	0.67	1.12
0.049	2. BD ( 1) N 1 - C 5	/403. BD*( 1) C 2 - B 6	2.47	1.17
0.023	2. BD ( 1) N 1 - C 5	/405. BD*( 1) N 3 - C 9	0.69	1.00
0.022	2. BD ( 1) N 1 - C 5	/406. BD*( 1) C 4 - C 5	0.52	1.21
0.053	2. BD ( 1) N 1 - C 5	/408. BD*( 1) C 4 - H 19	3.36	1.06
0.039	3. BD ( 1) N 1 - C 10	/ 80. RY*( 1) C 2	0.75	2.51
0.033	3. BD ( 1) N 1 - C 10	/123. RY*( 2) C 5	0.63	2.12
0.026	3. BD ( 1) N 1 - C 10	/398. BD*( 1) N 1 - C 2	0.80	1.08
0.038	3. BD ( 1) N 1 - C 10	/401. BD*( 1) C 2 - N 3	1.69	1.08
0.027	3. BD ( 1) N 1 - C 10	/406. BD*( 1) C 4 - C 5	0.80	1.18
0.032	4. BD ( 1) C 2 - N 3	/109. RY*( 2) C 4	0.58	2.15
0.060	4. BD ( 1) C 2 - N 3	/400. BD*( 1) N 1 - C 10	4.55	0.99
0.040	4. BD ( 1) C 2 - N 3	/403. BD*( 1) C 2 - B 6	1.69	1.17
0.029	4. BD ( 1) C 2 - N 3	/404. BD*( 1) N 3 - C 4	0.97	1.09
0.020	4. BD ( 1) C 2 - N 3	/405. BD*( 1) N 3 - C 9	0.50	1.00

0.046	4. BD ( 1) C 2 - N 3	/408. BD*( 1) C 4 - H 19	2.56	1.05
0.026	4. BD ( 1) C 2 - N 3	/411. BD*( 1) B 6 - B 11	0.67	1.25
0.043	5. BD ( 2) C 2 - N 3	/ 61. LP ( 1) B 6	4.86	0.34
0.043	5. BD ( 2) C 2 - N 3	/108. RY*( 1) C 4	2.45	0.86
0.062	5. BD ( 2) C 2 - N 3	/407. BD*( 2) C 4 - C 5	16.76	0.27
0.038	5. BD ( 2) C 2 - N 3	/415. BD*( 1) C 9 - H 32	2.87	0.60
0.040	5. BD ( 2) C 2 - N 3	/416. BD*( 1) C 9 - H 33	3.13	0.60
0.048	6. BD ( 1) C 2 - B 6	/ 66. RY*( 1) N 1	1.32	2.16
0.036	6. BD ( 1) C 2 - B 6	/ 80. RY*( 1) C 2	0.68	2.31
0.048	6. BD ( 1) C 2 - B 6	/ 94. RY*( 1) N 3	1.33	2.16
0.027	6. BD ( 1) C 2 - B 6	/ 96. RY*( 3) N 3	0.51	1.74
0.127	6. BD ( 1) C 2 - B 6	/148. RY*( 13) B 6	1.71	11.65
0.061	6. BD ( 1) C 2 - B 6	/206. RY*( 1) B 11	2.63	1.76
0.031	6. BD ( 1) C 2 - B 6	/208. RY*( 3) B 11	0.51	2.28
0.030	6. BD ( 1) C 2 - B 6	/398. BD*( 1) N 1 - C 2	1.32	0.87
0.049	6. BD ( 1) C 2 - B 6	/399. BD*( 1) N 1 - C 5	3.51	0.85
0.032	6. BD ( 1) C 2 - B 6	/401. BD*( 1) C 2 - N 3	1.43	0.87
0.050	6. BD ( 1) C 2 - B 6	/404. BD*( 1) N 3 - C 4	3.60	0.85
0.040	6. BD ( 1) C 2 - B 6	/410. BD*( 1) B 6 - C 7	2.08	0.97
0.061	6. BD ( 1) C 2 - B 6	/411. BD*( 1) B 6 - B 11	4.59	1.01
0.029	6. BD ( 1) C 2 - B 6	/412. BD*( 1) C 7 - O 8	1.00	1.04
0.031	6. BD ( 1) C 2 - B 6	/414. BD*( 1) C 7 - B 11	1.34	0.86
0.035	6. BD ( 1) C 2 - B 6	/421. BD*( 1) B 11 - C 12	1.61	0.95
0.045	7. BD ( 1) N 3 - C 4	/ 80. RY*( 1) C 2	1.00	2.55
0.031	7. BD ( 1) N 3 - C 4	/ 83. RY*( 4) C 2	0.61	1.99
0.028	7. BD ( 1) N 3 - C 4	/180. RY*( 3) C 9	0.64	1.58
0.025	7. BD ( 1) N 3 - C 4	/398. BD*( 1) N 1 - C 2	0.67	1.11
0.024	7. BD ( 1) N 3 - C 4	/400. BD*( 1) N 1 - C 10	0.70	0.99
0.028	7. BD ( 1) N 3 - C 4	/401. BD*( 1) C 2 - N 3	0.84	1.11
0.049	7. BD ( 1) N 3 - C 4	/403. BD*( 1) C 2 - B 6	2.51	1.17
0.023	7. BD ( 1) N 3 - C 4	/406. BD*( 1) C 4 - C 5	0.53	1.21
0.053	7. BD ( 1) N 3 - C 4	/409. BD*( 1) C 5 - H 20	3.37	1.05
0.040	8. BD ( 1) N 3 - C 9	/ 80. RY*( 1) C 2	0.82	2.50
0.032	8. BD ( 1) N 3 - C 9	/109. RY*( 2) C 4	0.62	2.10
0.039	8. BD ( 1) N 3 - C 9	/398. BD*( 1) N 1 - C 2	1.73	1.07

0.026	8. BD ( 1) N 3 - C 9	/401. BD*( 1) C 2 - N 3	0.78	1.07
0.028	8. BD ( 1) N 3 - C 9	/406. BD*( 1) C 4 - C 5	0.87	1.17
0.043	9. BD ( 1) C 4 - C 5	/ 66. RY*( 1) N 1	0.98	2.33
0.042	9. BD ( 1) C 4 - C 5	/ 94. RY*( 1) N 3	0.96	2.32
0.062	9. BD ( 1) C 4 - C 5	/400. BD*( 1) N 1 - C 10	5.26	0.92
0.061	9. BD ( 1) C 4 - C 5	/405. BD*( 1) N 3 - C 9	5.10	0.92
0.026	9. BD ( 1) C 4 - C 5	/408. BD*( 1) C 4 - H 19	0.83	0.98
0.026	9. BD ( 1) C 4 - C 5	/409. BD*( 1) C 5 - H 20	0.84	0.98
0.041	10. BD ( 2) C 4 - C 5	/402. BD*( 2) C 2 - N 3	7.71	0.21
0.047	11. BD ( 1) C 4 - H 19	/ 94. RY*( 1) N 3	1.28	2.16
0.042	11. BD ( 1) C 4 - H 19	/123. RY*( 2) C 5	1.15	1.92
0.035	11. BD ( 1) C 4 - H 19	/399. BD*( 1) N 1 - C 5	1.81	0.86
0.051	11. BD ( 1) C 4 - H 19	/401. BD*( 1) C 2 - N 3	3.72	0.88
0.022	11. BD ( 1) C 4 - H 19	/406. BD*( 1) C 4 - C 5	0.61	0.98
0.047	12. BD ( 1) C 5 - H 20	/ 66. RY*( 1) N 1	1.26	2.17
0.042	12. BD ( 1) C 5 - H 20	/109. RY*( 2) C 4	1.17	1.92
0.051	12. BD ( 1) C 5 - H 20	/398. BD*( 1) N 1 - C 2	3.71	0.88
0.035	12. BD ( 1) C 5 - H 20	/404. BD*( 1) N 3 - C 4	1.81	0.86
0.022	12. BD ( 1) C 5 - H 20	/406. BD*( 1) C 4 - C 5	0.62	0.98
0.024	13. BD ( 1) B 6 - C 7	/ 61. LP ( 1) B 6	1.13	0.42
0.051	13. BD ( 1) B 6 - C 7	/ 80. RY*( 1) C 2	1.41	2.19
0.027	13. BD ( 1) B 6 - C 7	/138. RY*( 3) B 6	0.55	1.60
0.044	13. BD ( 1) B 6 - C 7	/142. RY*( 7) B 6	0.73	3.15
0.040	13. BD ( 1) B 6 - C 7	/143. RY*( 8) B 6	0.72	2.63
0.124	13. BD ( 1) B 6 - C 7	/148. RY*( 13) B 6	1.59	11.54
0.040	13. BD ( 1) B 6 - C 7	/164. RY*( 1) O 8	1.63	1.16
0.040	13. BD ( 1) B 6 - C 7	/166. RY*( 3) O 8	1.29	1.50
0.029	13. BD ( 1) B 6 - C 7	/206. RY*( 1) B 11	0.63	1.64
0.042	13. BD ( 1) B 6 - C 7	/207. RY*( 2) B 11	1.16	1.79
0.031	13. BD ( 1) B 6 - C 7	/208. RY*( 3) B 11	0.52	2.16
0.029	13. BD ( 1) B 6 - C 7	/209. RY*( 4) B 11	0.70	1.41
0.049	13. BD ( 1) B 6 - C 7	/398. BD*( 1) N 1 - C 2	3.90	0.76
0.049	13. BD ( 1) B 6 - C 7	/403. BD*( 1) C 2 - B 6	3.61	0.81
0.026	13. BD ( 1) B 6 - C 7	/410. BD*( 1) B 6 - C 7	0.96	0.85
0.060	13. BD ( 1) B 6 - C 7	/411. BD*( 1) B 6 - B 11	4.94	0.89



0.035	13. BD ( 1) B 6 - C 7	/412. BD*( 1) C 7 - O 8	1.61	0.92
0.060	13. BD ( 1) B 6 - C 7	/414. BD*( 1) C 7 - B 11	5.97	0.75
0.104	13. BD ( 1) B 6 - C 7	/421. BD*( 1) B 11 - C 12	15.60	0.84
0.018	14. BD ( 1) B 6 - B 11	/ 61. LP ( 1) B 6	0.92	0.31
0.062	14. BD ( 1) B 6 - B 11	/ 80. RY*( 1) C 2	2.15	2.08
0.029	14. BD ( 1) B 6 - B 11	/ 82. RY*( 3) C 2	0.58	1.67
0.035	14. BD ( 1) B 6 - B 11	/136. RY*( 1) B 6	0.63	2.29
0.115	14. BD ( 1) B 6 - B 11	/148. RY*( 13) B 6	1.32	11.43
0.028	14. BD ( 1) B 6 - B 11	/150. RY*( 1) C 7	0.80	1.13
0.042	14. BD ( 1) B 6 - B 11	/206. RY*( 1) B 11	1.35	1.53
0.029	14. BD ( 1) B 6 - B 11	/210. RY*( 5) B 11	0.66	1.44
0.069	14. BD ( 1) B 6 - B 11	/220. RY*( 1) C 12	2.64	2.09
0.030	14. BD ( 1) B 6 - B 11	/223. RY*( 4) C 12	0.61	1.65
0.049	14. BD ( 1) B 6 - B 11	/401. BD*( 1) C 2 - N 3	4.35	0.65
0.046	14. BD ( 1) B 6 - B 11	/403. BD*( 1) C 2 - B 6	3.62	0.70
0.043	14. BD ( 1) B 6 - B 11	/410. BD*( 1) B 6 - C 7	3.03	0.74
0.126	14. BD ( 1) B 6 - B 11	/412. BD*( 1) C 7 - O 8	22.92	0.81
0.042	14. BD ( 1) B 6 - B 11	/414. BD*( 1) C 7 - B 11	3.38	0.64
0.025	14. BD ( 1) B 6 - B 11	/419. BD*( 1) C 10 - H 30	1.18	0.60
0.037	14. BD ( 1) B 6 - B 11	/421. BD*( 1) B 11 - C 12	2.25	0.73
0.037	14. BD ( 1) B 6 - B 11	/422. BD*( 1) C 12 - N 13	2.49	0.65
0.017	14. BD ( 1) B 6 - B 11	/423. BD*( 2) C 12 - N 13	1.10	0.25
0.041	15. BD ( 1) C 7 - O 8	/150. RY*( 1) C 7	1.19	1.73
0.041	15. BD ( 1) C 7 - O 8	/410. BD*( 1) B 6 - C 7	1.56	1.33
0.038	15. BD ( 1) C 7 - O 8	/414. BD*( 1) C 7 - B 11	1.42	1.23
0.035	16. BD ( 2) C 7 - O 8	/ 61. LP ( 1) B 6	3.41	0.29
0.029	16. BD ( 2) C 7 - O 8	/ 64. LP*( 1) B 11	2.56	0.28
0.016	16. BD ( 2) C 7 - O 8	/413. BD*( 2) C 7 - O 8	0.85	0.31
0.041	17. BD ( 1) C 7 - B 11	/ 61. LP ( 1) B 6	4.46	0.35
0.029	17. BD ( 1) C 7 - B 11	/138. RY*( 3) B 6	0.60	1.52
0.035	17. BD ( 1) C 7 - B 11	/153. RY*( 4) C 7	0.61	2.17
0.033	17. BD ( 1) C 7 - B 11	/164. RY*( 1) O 8	1.11	1.09
0.032	17. BD ( 1) C 7 - B 11	/166. RY*( 3) O 8	0.77	1.42
0.026	17. BD ( 1) C 7 - B 11	/226. RY*( 7) C 12	0.50	1.49
0.140	17. BD ( 1) C 7 - B 11	/403. BD*( 1) C 2 - B 6	30.18	0.74

17.080	17. BD ( 1) C 7 - B 11	/410. BD*( 1) B 6 - C 7	9.38	0.77
0.079	17. BD ( 1) C 7 - B 11	/411. BD*( 1) B 6 - B 11	8.52	0.82
0.031	17. BD ( 1) C 7 - B 11	/414. BD*( 1) C 7 - B 11	1.71	0.67
0.024	17. BD ( 1) C 7 - B 11	/421. BD*( 1) B 11 - C 12	0.83	0.76
0.041	17. BD ( 1) C 7 - B 11	/423. BD*( 2) C 12 - N 13	5.83	0.28
0.038	17. BD ( 1) C 7 - B 11	/424. BD*( 1) C 12 - N 16	2.33	0.68
0.043	18. BD ( 1) C 9 - H 32	/401. BD*( 1) C 2 - N 3	2.75	0.83
0.027	18. BD ( 1) C 9 - H 32	/402. BD*( 2) C 2 - N 3	1.55	0.41
0.022	19. BD ( 1) C 9 - H 33	/ 95. RY*( 2) N 3	0.57	1.04
0.041	19. BD ( 1) C 9 - H 33	/401. BD*( 1) C 2 - N 3	2.46	0.83
0.028	19. BD ( 1) C 9 - H 33	/402. BD*( 2) C 2 - N 3	1.72	0.41
0.032	20. BD ( 1) C 9 - H 34	/ 96. RY*( 3) N 3	0.76	1.68
0.058	20. BD ( 1) C 9 - H 34	/404. BD*( 1) N 3 - C 4	5.21	0.79
0.043	21. BD ( 1) C 10 - H 29	/398. BD*( 1) N 1 - C 2	2.67	0.84
0.035	22. BD ( 1) C 10 - H 30	/ 68. RY*( 3) N 1	0.86	1.77
0.059	22. BD ( 1) C 10 - H 30	/399. BD*( 1) N 1 - C 5	5.39	0.80
0.020	22. BD ( 1) C 10 - H 30	/410. BD*( 1) B 6 - C 7	0.54	0.92
0.023	23. BD ( 1) C 10 - H 31	/ 67. RY*( 2) N 1	0.62	1.04
0.040	23. BD ( 1) C 10 - H 31	/398. BD*( 1) N 1 - C 2	2.31	0.84
0.091	24. BD ( 1) B 11 - C 12	/136. RY*( 1) B 6	4.07	2.52
0.029	24. BD ( 1) B 11 - C 12	/139. RY*( 4) B 6	0.71	1.51
0.026	24. BD ( 1) B 11 - C 12	/140. RY*( 5) B 6	0.57	1.50
0.054	24. BD ( 1) B 11 - C 12	/142. RY*( 7) B 6	1.10	3.27
0.033	24. BD ( 1) B 11 - C 12	/206. RY*( 1) B 11	0.75	1.76
0.045	24. BD ( 1) B 11 - C 12	/207. RY*( 2) B 11	1.32	1.91
0.057	24. BD ( 1) B 11 - C 12	/208. RY*( 3) B 11	1.77	2.28
0.029	24. BD ( 1) B 11 - C 12	/209. RY*( 4) B 11	0.69	1.52
0.052	24. BD ( 1) B 11 - C 12	/212. RY*( 7) B 11	1.20	2.74
0.096	24. BD ( 1) B 11 - C 12	/217. RY*( 12) B 11	1.64	6.87
0.031	24. BD ( 1) B 11 - C 12	/220. RY*( 1) C 12	0.52	2.32
0.033	24. BD ( 1) B 11 - C 12	/234. RY*( 1) N 13	0.77	1.78
0.042	24. BD ( 1) B 11 - C 12	/235. RY*( 2) N 13	1.32	1.62
0.050	24. BD ( 1) B 11 - C 12	/276. RY*( 1) N 16	1.51	2.07
0.023	24. BD ( 1) B 11 - C 12	/403. BD*( 1) C 2 - B 6	0.70	0.93
0.032	24. BD ( 1) B 11 - C 12	/410. BD*( 1) B 6 - C 7	1.34	0.97

24. BD ( 1) B 11 - C 12	/411. BD*( 1) B 6 - B 11	3.36	1.01
0.052			
24. BD ( 1) B 11 - C 12	/414. BD*( 1) C 7 - B 11	1.11	0.87
0.028			
24. BD ( 1) B 11 - C 12	/422. BD*( 1) C 12 - N 13	1.52	0.88
0.033			
24. BD ( 1) B 11 - C 12	/424. BD*( 1) C 12 - N 16	1.60	0.87
0.033			
24. BD ( 1) B 11 - C 12	/425. BD*( 1) N 13 - C 14	3.35	0.87
0.048			
24. BD ( 1) B 11 - C 12	/430. BD*( 1) C 15 - N 16	3.26	0.86
0.047			
25. BD ( 1) C 12 - N 13	/249. RY*( 2) C 14	0.59	2.07
0.031			
25. BD ( 1) C 12 - N 13	/250. RY*( 3) C 14	0.53	1.99
0.029			
25. BD ( 1) C 12 - N 13	/291. RY*( 2) C 17	0.62	1.63
0.028			
25. BD ( 1) C 12 - N 13	/411. BD*( 1) B 6 - B 11	0.93	1.22
0.030			
25. BD ( 1) C 12 - N 13	/421. BD*( 1) B 11 - C 12	1.89	1.17
0.042			
25. BD ( 1) C 12 - N 13	/425. BD*( 1) N 13 - C 14	0.86	1.08
0.027			
25. BD ( 1) C 12 - N 13	/429. BD*( 1) C 14 - H 21	2.59	1.04
0.047			
25. BD ( 1) C 12 - N 13	/432. BD*( 1) N 16 - C 18	4.43	0.99
0.059			
25. BD ( 1) C 12 - N 13	/433. BD*( 1) C 17 - H 23	0.59	1.02
0.022			
26. BD ( 2) C 12 - N 13	/ 64. LP*( 1) B 11	1.55	0.31
0.022			
26. BD ( 2) C 12 - N 13	/248. RY*( 1) C 14	2.27	0.94
0.043			
26. BD ( 2) C 12 - N 13	/290. RY*( 1) C 17	1.08	1.13
0.032			
26. BD ( 2) C 12 - N 13	/414. BD*( 1) C 7 - B 11	1.34	0.64
0.026			
26. BD ( 2) C 12 - N 13	/428. BD*( 2) C 14 - C 15	16.99	0.27
0.062			
26. BD ( 2) C 12 - N 13	/433. BD*( 1) C 17 - H 23	0.53	0.58
0.016			
26. BD ( 2) C 12 - N 13	/434. BD*( 1) C 17 - H 24	4.01	0.58
0.045			
26. BD ( 2) C 12 - N 13	/435. BD*( 1) C 17 - H 25	1.38	0.61
0.027			
27. BD ( 1) C 12 - N 16	/ 64. LP*( 1) B 11	0.51	0.75
0.021			
27. BD ( 1) C 12 - N 16	/263. RY*( 2) C 15	0.55	2.13
0.031			
27. BD ( 1) C 12 - N 16	/264. RY*( 3) C 15	0.53	1.99
0.029			
27. BD ( 1) C 12 - N 16	/305. RY*( 2) C 18	0.65	1.56
0.028			
27. BD ( 1) C 12 - N 16	/421. BD*( 1) B 11 - C 12	1.76	1.17
0.041			
27. BD ( 1) C 12 - N 16	/426. BD*( 1) N 13 - C 17	4.31	0.99
0.058			
27. BD ( 1) C 12 - N 16	/430. BD*( 1) C 15 - N 16	0.87	1.08
0.027			
27. BD ( 1) C 12 - N 16	/431. BD*( 1) C 15 - H 22	2.53	1.04
0.046			
28. BD ( 1) N 13 - C 14	/220. RY*( 1) C 12	0.66	2.54
0.037			
28. BD ( 1) N 13 - C 14	/224. RY*( 5) C 12	0.59	2.35
0.033			
28. BD ( 1) N 13 - C 14	/292. RY*( 3) C 17	0.56	1.97
0.030			
28. BD ( 1) N 13 - C 14	/421. BD*( 1) B 11 - C 12	2.42	1.18
0.048			

0.027	28. BD ( 1) N 13 - C 14	/422. BD* ( 1) C 12 - N 13	0.83	1.10
0.024	28. BD ( 1) N 13 - C 14	/424. BD* ( 1) C 12 - N 16	0.64	1.09
0.024	28. BD ( 1) N 13 - C 14	/427. BD* ( 1) C 14 - C 15	0.58	1.22
0.054	28. BD ( 1) N 13 - C 14	/431. BD* ( 1) C 15 - H 22	3.44	1.05
0.023	28. BD ( 1) N 13 - C 14	/432. BD* ( 1) N 16 - C 18	0.67	0.99
0.034	29. BD ( 1) N 13 - C 17	/220. RY* ( 1) C 12	0.58	2.50
0.030	29. BD ( 1) N 13 - C 17	/249. RY* ( 2) C 14	0.56	2.04
0.025	29. BD ( 1) N 13 - C 17	/422. BD* ( 1) C 12 - N 13	0.73	1.06
0.037	29. BD ( 1) N 13 - C 17	/424. BD* ( 1) C 12 - N 16	1.62	1.06
0.028	29. BD ( 1) N 13 - C 17	/427. BD* ( 1) C 14 - C 15	0.80	1.18
0.036	30. BD ( 1) C 14 - C 15	/234. RY* ( 1) N 13	0.83	1.93
0.039	30. BD ( 1) C 14 - C 15	/276. RY* ( 1) N 16	0.87	2.22
0.062	30. BD ( 1) C 14 - C 15	/426. BD* ( 1) N 13 - C 17	5.24	0.93
0.026	30. BD ( 1) C 14 - C 15	/429. BD* ( 1) C 14 - H 21	0.87	0.98
0.027	30. BD ( 1) C 14 - C 15	/431. BD* ( 1) C 15 - H 22	0.90	0.98
0.062	30. BD ( 1) C 14 - C 15	/432. BD* ( 1) N 16 - C 18	5.17	0.93
0.040	31. BD ( 2) C 14 - C 15	/423. BD* ( 2) C 12 - N 13	6.64	0.21
0.037	32. BD ( 1) C 14 - H 21	/234. RY* ( 1) N 13	0.95	1.77
0.029	32. BD ( 1) C 14 - H 21	/235. RY* ( 2) N 13	0.64	1.61
0.042	32. BD ( 1) C 14 - H 21	/263. RY* ( 2) C 15	1.15	1.90
0.050	32. BD ( 1) C 14 - H 21	/422. BD* ( 1) C 12 - N 13	3.63	0.87
0.023	32. BD ( 1) C 14 - H 21	/427. BD* ( 1) C 14 - C 15	0.67	0.98
0.036	32. BD ( 1) C 14 - H 21	/430. BD* ( 1) C 15 - N 16	1.90	0.85
0.046	33. BD ( 1) C 15 - N 16	/220. RY* ( 1) C 12	1.02	2.53
0.028	33. BD ( 1) C 15 - N 16	/222. RY* ( 3) C 12	0.53	1.89
0.031	33. BD ( 1) C 15 - N 16	/306. RY* ( 3) C 18	0.62	1.95
0.048	33. BD ( 1) C 15 - N 16	/421. BD* ( 1) B 11 - C 12	2.45	1.17
0.024	33. BD ( 1) C 15 - N 16	/422. BD* ( 1) C 12 - N 13	0.67	1.09
0.026	33. BD ( 1) C 15 - N 16	/424. BD* ( 1) C 12 - N 16	0.79	1.09
0.023	33. BD ( 1) C 15 - N 16	/426. BD* ( 1) N 13 - C 17	0.67	0.99
0.023	33. BD ( 1) C 15 - N 16	/427. BD* ( 1) C 14 - C 15	0.55	1.21
0.054	33. BD ( 1) C 15 - N 16	/429. BD* ( 1) C 14 - H 21	3.47	1.05
0.021	33. BD ( 1) C 15 - N 16	/438. BD* ( 1) C 18 - H 28	0.53	1.03
0.041	34. BD ( 1) C 15 - H 22	/249. RY* ( 2) C 14	1.11	1.84
0.043	34. BD ( 1) C 15 - H 22	/276. RY* ( 1) N 16	1.11	2.06

34. BD ( 1) C 15 - H 22	/424. BD*( 1) C 12 - N 16	3.59	0.86
0.050			
34. BD ( 1) C 15 - H 22	/425. BD*( 1) N 13 - C 14	1.90	0.86
0.036			
34. BD ( 1) C 15 - H 22	/427. BD*( 1) C 14 - C 15	0.70	0.99
0.023			
35. BD ( 1) N 16 - C 18	/220. RY*( 1) C 12	0.62	2.51
0.035			
35. BD ( 1) N 16 - C 18	/263. RY*( 2) C 15	0.63	2.11
0.032			
35. BD ( 1) N 16 - C 18	/422. BD*( 1) C 12 - N 13	1.50	1.07
0.036			
35. BD ( 1) N 16 - C 18	/424. BD*( 1) C 12 - N 16	0.71	1.07
0.025			
35. BD ( 1) N 16 - C 18	/427. BD*( 1) C 14 - C 15	0.78	1.19
0.027			
36. BD ( 1) C 17 - H 23	/236. RY*( 3) N 13	0.89	1.72
0.035			
36. BD ( 1) C 17 - H 23	/422. BD*( 1) C 12 - N 13	4.80	0.83
0.057			
37. BD ( 1) C 17 - H 24	/423. BD*( 2) C 12 - N 13	1.63	0.42
0.029			
37. BD ( 1) C 17 - H 24	/425. BD*( 1) N 13 - C 14	1.37	0.81
0.030			
38. BD ( 1) C 17 - H 25	/423. BD*( 2) C 12 - N 13	0.82	0.41
0.020			
38. BD ( 1) C 17 - H 25	/425. BD*( 1) N 13 - C 14	3.77	0.80
0.049			
39. BD ( 1) C 18 - H 26	/424. BD*( 1) C 12 - N 16	3.79	0.83
0.050			
40. BD ( 1) C 18 - H 27	/424. BD*( 1) C 12 - N 16	1.28	0.82
0.029			
41. BD ( 1) C 18 - H 28	/ 64. LP*( 1) B 11	0.64	0.49
0.019			
41. BD ( 1) C 18 - H 28	/278. RY*( 3) N 16	0.79	1.77
0.033			
41. BD ( 1) C 18 - H 28	/430. BD*( 1) C 15 - N 16	4.96	0.81
0.057			
42. CR ( 1) N 1	/ 83. RY*( 4) C 2	1.42	15.11
0.131			
42. CR ( 1) N 1	/124. RY*( 3) C 5	1.40	15.12
0.130			
42. CR ( 1) N 1	/194. RY*( 3) C 10	0.86	15.13
0.102			
42. CR ( 1) N 1	/403. BD*( 1) C 2 - B 6	0.58	14.29
0.083			
43. CR ( 1) C 2	/137. RY*( 2) B 6	0.72	11.15
0.080			
43. CR ( 1) C 2	/399. BD*( 1) N 1 - C 5	0.54	10.13
0.067			
43. CR ( 1) C 2	/400. BD*( 1) N 1 - C 10	1.03	10.04
0.091			
43. CR ( 1) C 2	/403. BD*( 1) C 2 - B 6	1.83	10.22
0.124			
43. CR ( 1) C 2	/404. BD*( 1) N 3 - C 4	0.53	10.14
0.066			
43. CR ( 1) C 2	/405. BD*( 1) N 3 - C 9	1.04	10.04
0.092			
43. CR ( 1) C 2	/410. BD*( 1) B 6 - C 7	0.59	10.25
0.071			
43. CR ( 1) C 2	/411. BD*( 1) B 6 - B 11	1.04	10.29
0.093			
44. CR ( 1) N 3	/ 83. RY*( 4) C 2	0.69	15.11
0.091			
44. CR ( 1) N 3	/110. RY*( 3) C 4	1.40	15.13
0.130			
44. CR ( 1) N 3	/180. RY*( 3) C 9	0.58	14.71
0.082			
44. CR ( 1) N 3	/403. BD*( 1) C 2 - B 6	0.57	14.29
0.082			

0.073	45. CR ( 1) C 4	/ 96. RY*( ( 3) N 3	0.60	11.03
0.108	45. CR ( 1) C 4	/123. RY*( ( 2) C 5	1.30	11.20
0.070	45. CR ( 1) C 4	/401. BD*( ( 1) C 2 - N 3	0.59	10.16
0.092	45. CR ( 1) C 4	/405. BD*( ( 1) N 3 - C 9	1.04	10.04
0.089	45. CR ( 1) C 4	/406. BD*( ( 1) C 4 - C 5	0.97	10.25
0.088	45. CR ( 1) C 4	/409. BD*( ( 1) C 5 - H 20	0.96	10.09
0.069	46. CR ( 1) C 5	/ 68. RY*( ( 3) N 1	0.54	11.10
0.109	46. CR ( 1) C 5	/109. RY*( ( 2) C 4	1.33	11.19
0.069	46. CR ( 1) C 5	/398. BD*( ( 1) N 1 - C 2	0.58	10.16
0.093	46. CR ( 1) C 5	/400. BD*( ( 1) N 1 - C 10	1.08	10.04
0.090	46. CR ( 1) C 5	/406. BD*( ( 1) C 4 - C 5	0.99	10.26
0.088	46. CR ( 1) C 5	/408. BD*( ( 1) C 4 - H 19	0.95	10.10
0.076	47. CR ( 1) B 6	/ 80. RY*( ( 1) C 2	0.89	8.10
0.084	47. CR ( 1) B 6	/150. RY*( ( 1) C 7	1.22	7.15
0.058	47. CR ( 1) B 6	/153. RY*( ( 4) C 7	0.51	8.15
0.099	47. CR ( 1) B 6	/206. RY*( ( 1) B 11	1.61	7.55
0.090	47. CR ( 1) B 6	/398. BD*( ( 1) N 1 - C 2	1.50	6.66
0.083	47. CR ( 1) B 6	/401. BD*( ( 1) C 2 - N 3	1.26	6.66
0.056	47. CR ( 1) B 6	/410. BD*( ( 1) B 6 - C 7	0.57	6.76
0.092	47. CR ( 1) B 6	/411. BD*( ( 1) B 6 - B 11	1.54	6.80
0.148	47. CR ( 1) B 6	/412. BD*( ( 1) C 7 - O 8	3.92	6.83
0.080	47. CR ( 1) B 6	/414. BD*( ( 1) C 7 - B 11	1.13	6.65
0.158	47. CR ( 1) B 6	/421. BD*( ( 1) B 11 - C 12	4.55	6.74
0.078	48. CR ( 1) C 7	/167. RY*( ( 4) O 8	0.70	10.94
0.069	48. CR ( 1) C 7	/206. RY*( ( 1) B 11	0.55	10.98
0.146	48. CR ( 1) C 7	/403. BD*( ( 1) C 2 - B 6	2.58	10.15
0.121	48. CR ( 1) C 7	/410. BD*( ( 1) B 6 - C 7	1.75	10.19
0.092	48. CR ( 1) C 7	/412. BD*( ( 1) C 7 - O 8	1.02	10.26
0.082	48. CR ( 1) C 7	/414. BD*( ( 1) C 7 - B 11	0.78	10.08
0.087	48. CR ( 1) C 7	/421. BD*( ( 1) B 11 - C 12	0.92	10.17
0.283	49. CR ( 1) O 8	/150. RY*( ( 1) C 7	5.17	19.25
0.120	49. CR ( 1) O 8	/410. BD*( ( 1) B 6 - C 7	0.93	18.85
0.115	49. CR ( 1) O 8	/414. BD*( ( 1) C 7 - B 11	0.83	18.75
0.081	50. CR ( 1) C 9	/401. BD*( ( 1) C 2 - N 3	0.80	10.15
0.078	50. CR ( 1) C 9	/404. BD*( ( 1) N 3 - C 4	0.75	10.13

0.075	50. CR ( 1) C 9	/405. BD*( 1) N 3 - C 9	0.69	10.03
0.080	51. CR ( 1) C 10	/398. BD*( 1) N 1 - C 2	0.77	10.16
0.080	51. CR ( 1) C 10	/399. BD*( 1) N 1 - C 5	0.78	10.13
0.070	51. CR ( 1) C 10	/400. BD*( 1) N 1 - C 10	0.60	10.04
0.083	52. CR ( 1) B 11	/136. RY*( 1) B 6	1.03	8.32
0.054	52. CR ( 1) B 11	/150. RY*( 1) C 7	0.50	7.16
0.073	52. CR ( 1) B 11	/220. RY*( 1) C 12	0.82	8.11
0.152	52. CR ( 1) B 11	/403. BD*( 1) C 2 - B 6	4.18	6.73
0.079	52. CR ( 1) B 11	/410. BD*( 1) B 6 - C 7	1.11	6.77
0.089	52. CR ( 1) B 11	/411. BD*( 1) B 6 - B 11	1.43	6.81
0.102	52. CR ( 1) B 11	/412. BD*( 1) C 7 - O 8	1.87	6.84
0.060	52. CR ( 1) B 11	/414. BD*( 1) C 7 - B 11	0.63	6.66
0.083	52. CR ( 1) B 11	/422. BD*( 1) C 12 - N 13	1.26	6.68
0.094	52. CR ( 1) B 11	/424. BD*( 1) C 12 - N 16	1.61	6.67
0.103	53. CR ( 1) C 12	/206. RY*( 1) B 11	1.20	11.03
0.077	53. CR ( 1) C 12	/210. RY*( 5) B 11	0.68	10.94
0.118	53. CR ( 1) C 12	/411. BD*( 1) B 6 - B 11	1.67	10.28
0.130	53. CR ( 1) C 12	/421. BD*( 1) B 11 - C 12	2.03	10.22
0.065	53. CR ( 1) C 12	/425. BD*( 1) N 13 - C 14	0.51	10.14
0.088	53. CR ( 1) C 12	/426. BD*( 1) N 13 - C 17	0.96	10.05
0.064	53. CR ( 1) C 12	/430. BD*( 1) C 15 - N 16	0.51	10.13
0.090	53. CR ( 1) C 12	/432. BD*( 1) N 16 - C 18	1.01	10.04
0.109	54. CR ( 1) N 13	/224. RY*( 5) C 12	0.97	15.47
0.130	54. CR ( 1) N 13	/250. RY*( 3) C 14	1.41	15.12
0.106	54. CR ( 1) N 13	/292. RY*( 3) C 17	0.93	15.09
0.085	54. CR ( 1) N 13	/421. BD*( 1) B 11 - C 12	0.63	14.30
0.070	55. CR ( 1) C 14	/236. RY*( 3) N 13	0.55	11.04
0.110	55. CR ( 1) C 14	/263. RY*( 2) C 15	1.36	11.18
0.068	55. CR ( 1) C 14	/422. BD*( 1) C 12 - N 13	0.56	10.14
0.095	55. CR ( 1) C 14	/426. BD*( 1) N 13 - C 17	1.12	10.04
0.092	55. CR ( 1) C 14	/427. BD*( 1) C 14 - C 15	1.03	10.26
0.090	55. CR ( 1) C 14	/431. BD*( 1) C 15 - H 22	0.99	10.09
0.108	56. CR ( 1) C 15	/249. RY*( 2) C 14	1.33	11.12
0.071	56. CR ( 1) C 15	/278. RY*( 3) N 16	0.58	11.08
0.068	56. CR ( 1) C 15	/424. BD*( 1) C 12 - N 16	0.55	10.14

56. CR ( 1) C 15	/427. BD*( 1) C 14 - C 15	1.05	10.26
0.093			
56. CR ( 1) C 15	/429. BD*( 1) C 14 - H 21	0.98	10.09
0.089			
56. CR ( 1) C 15	/432. BD*( 1) N 16 - C 18	1.08	10.04
0.093			
57. CR ( 1) N 16	/222. RY*( 3) C 12	1.08	15.02
0.114			
57. CR ( 1) N 16	/264. RY*( 3) C 15	1.35	15.12
0.127			
57. CR ( 1) N 16	/306. RY*( 3) C 18	0.97	15.07
0.108			
57. CR ( 1) N 16	/421. BD*( 1) B 11 - C 12	0.64	14.30
0.086			
58. CR ( 1) C 17	/422. BD*( 1) C 12 - N 13	0.75	10.14
0.079			
58. CR ( 1) C 17	/425. BD*( 1) N 13 - C 14	0.80	10.14
0.081			
58. CR ( 1) C 17	/426. BD*( 1) N 13 - C 17	0.61	10.04
0.070			
59. CR ( 1) C 18	/424. BD*( 1) C 12 - N 16	0.77	10.15
0.080			
59. CR ( 1) C 18	/430. BD*( 1) C 15 - N 16	0.77	10.14
0.080			
59. CR ( 1) C 18	/432. BD*( 1) N 16 - C 18	0.56	10.05
0.067			
60. LP ( 1) N 1	/ 85. RY*( 6) C 2	1.03	1.90
0.045			
60. LP ( 1) N 1	/122. RY*( 1) C 5	3.22	0.79
0.052			
60. LP ( 1) N 1	/192. RY*( 1) C 10	1.29	0.95
0.036			
60. LP ( 1) N 1	/402. BD*( 2) C 2 - N 3	52.57	0.19
0.093			
60. LP ( 1) N 1	/407. BD*( 2) C 4 - C 5	29.04	0.21
0.072			
60. LP ( 1) N 1	/418. BD*( 1) C 10 - H 29	4.15	0.52
0.048			
60. LP ( 1) N 1	/420. BD*( 1) C 10 - H 31	4.68	0.52
0.050			
61. LP ( 1) B 6	/ 86. RY*( 7) C 2	0.65	1.42
0.044			
61. LP ( 1) B 6	/140. RY*( 5) B 6	0.54	0.96
0.033			
61. LP ( 1) B 6	/151. RY*( 2) C 7	0.71	1.89
0.053			
61. LP ( 1) B 6	/410. BD*( 1) B 6 - C 7	1.74	0.43
0.038			
61. LP ( 1) B 6	/411. BD*( 1) B 6 - B 11	1.38	0.47
0.036			
61. LP ( 1) B 6	/413. BD*( 2) C 7 - O 8	215.59	0.03
0.089			
62. LP ( 1) O 8	/150. RY*( 1) C 7	12.59	1.41
0.119			
62. LP ( 1) O 8	/156. RY*( 7) C 7	0.74	1.98
0.035			
62. LP ( 1) O 8	/410. BD*( 1) B 6 - C 7	5.38	1.02
0.067			
62. LP ( 1) O 8	/414. BD*( 1) C 7 - B 11	2.97	0.92
0.048			
63. LP ( 2) O 8	/152. RY*( 3) C 7	1.67	2.39
0.060			
63. LP ( 2) O 8	/154. RY*( 5) C 7	1.05	1.48
0.037			
63. LP ( 2) O 8	/410. BD*( 1) B 6 - C 7	9.94	0.60
0.072			
63. LP ( 2) O 8	/414. BD*( 1) C 7 - B 11	19.18	0.50
0.090			
64. LP*( 1) B 11	/413. BD*( 2) C 7 - O 8	94.90	0.03
0.067			



0.066	64. LP* ( 1) B 11	/422. BD* ( 1) C 12 - N 13	5.27	0.34
0.073	64. LP* ( 1) B 11	/424. BD* ( 1) C 12 - N 16	6.56	0.33
0.049	65. LP ( 1) N 16	/225. RY* ( 6) C 12	1.17	1.99
0.050	65. LP ( 1) N 16	/262. RY* ( 1) C 15	3.25	0.76
0.038	65. LP ( 1) N 16	/304. RY* ( 1) C 18	1.31	1.06
0.091	65. LP ( 1) N 16	/423. BD* ( 2) C 12 - N 13	48.73	0.19
0.071	65. LP ( 1) N 16	/428. BD* ( 2) C 14 - C 15	28.97	0.20
0.038	65. LP ( 1) N 16	/436. BD* ( 1) C 18 - H 26	2.76	0.51
0.057	65. LP ( 1) N 16	/437. BD* ( 1) C 18 - H 27	6.30	0.51
0.017	65. LP ( 1) N 16	/438. BD* ( 1) C 18 - H 28	0.56	0.53
0.088	402. BD* ( 2) C 2 - N 3	/ 61. LP ( 1) B 6	81.07	0.08
0.011	402. BD* ( 2) C 2 - N 3	/ 64. LP* ( 1) B 11	1.18	0.08
0.087	402. BD* ( 2) C 2 - N 3	/ 81. RY* ( 2) C 2	2.38	1.17
0.038	402. BD* ( 2) C 2 - N 3	/ 95. RY* ( 2) N 3	0.87	0.62
0.071	402. BD* ( 2) C 2 - N 3	/ 98. RY* ( 5) N 3	0.81	2.26
0.029	402. BD* ( 2) C 2 - N 3	/108. RY* ( 1) C 4	0.53	0.60
0.038	402. BD* ( 2) C 2 - N 3	/407. BD* ( 2) C 4 - C 5	65.32	0.01
0.027	402. BD* ( 2) C 2 - N 3	/415. BD* ( 1) C 9 - H 32	0.83	0.34
0.029	402. BD* ( 2) C 2 - N 3	/416. BD* ( 1) C 9 - H 33	0.92	0.34
0.069	407. BD* ( 2) C 4 - C 5	/112. RY* ( 5) C 4	0.50	1.78
0.070	407. BD* ( 2) C 4 - C 5	/126. RY* ( 5) C 5	0.51	1.78
0.116	413. BD* ( 2) C 7 - O 8	/151. RY* ( 2) C 7	1.98	1.86
0.047	413. BD* ( 2) C 7 - O 8	/160. RY* ( 11) C 7	0.52	1.16
0.082	413. BD* ( 2) C 7 - O 8	/165. RY* ( 2) O 8	2.95	0.62
0.057	413. BD* ( 2) C 7 - O 8	/412. BD* ( 1) C 7 - O 8	2.05	0.47
0.135	414. BD* ( 1) C 7 - B 11	/152. RY* ( 3) C 7	0.71	1.89
0.102	414. BD* ( 1) C 7 - B 11	/208. RY* ( 3) B 11	0.54	1.42
0.077	414. BD* ( 1) C 7 - B 11	/210. RY* ( 5) B 11	0.54	0.81
0.086	414. BD* ( 1) C 7 - B 11	/411. BD* ( 1) B 6 - B 11	4.96	0.14
0.041	414. BD* ( 1) C 7 - B 11	/412. BD* ( 1) C 7 - O 8	0.97	0.18
0.038	414. BD* ( 1) C 7 - B 11	/422. BD* ( 1) C 12 - N 13	12.65	0.01
0.007	423. BD* ( 2) C 12 - N 13	/ 61. LP ( 1) B 6	0.69	0.07
0.050	423. BD* ( 2) C 12 - N 13	/ 64. LP* ( 1) B 11	33.77	0.06
0.075	423. BD* ( 2) C 12 - N 13	/221. RY* ( 2) C 12	1.74	1.41
0.056	423. BD* ( 2) C 12 - N 13	/223. RY* ( 4) C 12	0.97	1.41

0.063	423. BD* ( 2) C 12 - N 13	/238. RY* ( 5) N 13	0.78	2.23
0.029	423. BD* ( 2) C 12 - N 13	/248. RY* ( 1) C 14	0.53	0.69
0.035	423. BD* ( 2) C 12 - N 13	/411. BD* ( 1) B 6 - B 11	1.03	0.53
0.058	423. BD* ( 2) C 12 - N 13	/414. BD* ( 1) C 7 - B 11	4.39	0.39
0.037	423. BD* ( 2) C 12 - N 13	/428. BD* ( 2) C 14 - C 15	53.49	0.02
0.034	423. BD* ( 2) C 12 - N 13	/434. BD* ( 1) C 17 - H 24	1.59	0.33
0.023	423. BD* ( 2) C 12 - N 13	/435. BD* ( 1) C 17 - H 25	0.66	0.36
0.068	428. BD* ( 2) C 14 - C 15	/252. RY* ( 5) C 14	0.52	1.71

Natural Bond Orbitals (Summary):

NBO		Occupancy	Energy	Principal Delocalizations (geminal, vicinal, remote)
=====				
Molecular unit 1 (C11H16B2N4O)				
1.	BD ( 1) N 1 - C 2	1.98001	-0.75246	405 (v), 409 (v), 403 (g), 399 (g) 193 (v), 410 (v), 123 (v), 400 (g) 124 (v)
2.	BD ( 1) N 1 - C 5	1.98425	-0.75155	408 (v), 403 (v), 83 (v), 398 (g) 80 (v), 405 (r), 401 (v), 194 (v) 406 (g)
3.	BD ( 1) N 1 - C 10	1.99022	-0.71380	401 (v), 398 (g), 406 (v), 80 (v) 123 (v)
4.	BD ( 1) C 2 - N 3	1.98001	-0.75108	400 (v), 408 (v), 403 (g), 404 (g) 411 (v), 109 (v)
5.	BD ( 2) C 2 - N 3	1.85099	-0.30630	407 (v), 61 (v), 416 (v), 415 (v) 108 (v)
6.	BD ( 1) C 2 - B 6	1.96108	-0.50918	411 (g), 404 (v), 399 (v), 206 (g) 410 (g), 148 (g), 421 (v), 401 (g) 414 (v), 94 (v), 66 (v), 398 (g) 412 (v), 80 (g), 208 (v), 96 (v)
7.	BD ( 1) N 3 - C 4	1.98403	-0.74962	409 (v), 403 (v), 80 (v), 401 (g) 400 (r), 398 (v), 180 (v), 83 (v) 406 (g)
8.	BD ( 1) N 3 - C 9	1.98983	-0.70424	398 (v), 406 (v), 80 (v), 401 (g) 109 (v)
9.	BD ( 1) C 4 - C 5	1.97894	-0.67761	400 (v), 405 (v), 66 (v), 94 (v) 409 (g), 408 (g)
10.	BD ( 2) C 4 - C 5	1.87415	-0.26243	402 (v)
11.	BD ( 1) C 4 - H 19	1.98232	-0.51595	401 (v), 399 (v), 94 (v), 123 (v) 406 (g)
12.	BD ( 1) C 5 - H 20	1.98252	-0.51740	398 (v), 404 (v), 66 (v), 109 (v) 406 (g)
13.	BD ( 1) B 6 - C 7	1.89970	-0.39317	421 (v), 414 (g), 411 (g), 398 (v) 403 (g), 164 (v), 148 (g), 61 (g) 412 (g), 80 (v), 166 (v), 207 (v) 410 (g), 142 (g), 143 (g), 209 (v) 206 (v), 138 (g), 208 (v)
14.	BD ( 1) B 6 - B 11	1.82653	-0.28192	412 (v), 401 (v), 403 (g), 414 (g) 410 (g), 220 (v), 422 (v), 421 (g) 80 (v), 423 (v), 206 (g), 148 (g) 61 (g), 419 (r), 150 (v), 210 (g) 136 (g), 223 (v), 82 (v)
15.	BD ( 1) C 7 - O 8	1.99656	-0.87726	410 (g), 414 (g), 150 (g)
16.	BD ( 2) C 7 - O 8	1.98543	-0.25488	61 (v), 64 (v), 413 (g)
17.	BD ( 1) C 7 - B 11	1.74346	-0.31804	403 (v), 410 (g), 411 (g), 423 (v) 61 (v), 424 (v), 414 (g), 164 (v) 421 (g), 166 (v), 153 (g), 138 (v) 226 (v)
18.	BD ( 1) C 9 - H 32	1.98423	-0.46244	401 (v), 402 (v)
19.	BD ( 1) C 9 - H 33	1.98400	-0.46194	401 (v), 402 (v), 95 (v)
20.	BD ( 1) C 9 - H 34	1.98391	-0.45120	404 (v), 96 (v)

21. BD ( 1) C 10 - H 29	1.98512	-0.47339 398 (v)
22. BD ( 1) C 10 - H 30	1.98351	-0.46358 399 (v) , 68 (v) , 410 (r)
23. BD ( 1) C 10 - H 31	1.98503	-0.47311 398 (v) , 67 (v)
24. BD ( 1) B 11 - C 12	1.96884	-0.51114 136 (v) , 411 (g) , 425 (v) , 430 (g) 208 (g) , 217 (g) , 424 (g) , 422 (g) 276 (v) , 410 (v) , 207 (g) , 235 (v) 212 (g) , 414 (g) , 142 (v) , 234 (v) 206 (g) , 139 (v) , 403 (v) , 209 (g) 140 (v) , 220 (g)
25. BD ( 1) C 12 - N 13	1.97811	-0.72380 432 (v) , 429 (v) , 421 (g) , 411 (v) 425 (g) , 291 (v) , 433 (v) , 249 (v) 250 (v)
26. BD ( 2) C 12 - N 13	1.84802	-0.28557 428 (v) , 434 (v) , 248 (v) , 64 (v) 435 (v) , 414 (v) , 290 (v) , 433 (v)
27. BD ( 1) C 12 - N 16	1.97905	-0.72584 426 (v) , 431 (v) , 421 (g) , 430 (g) 64 (v) , 305 (v) , 263 (v) , 264 (v)
28. BD ( 1) N 13 - C 14	1.98342	-0.73160 431 (v) , 421 (v) , 422 (g) , 432 (r) 220 (v) , 424 (v) , 224 (v) , 427 (g) 292 (v)
29. BD ( 1) N 13 - C 17	1.99041	-0.69668 424 (v) , 427 (v) , 422 (g) , 220 (v) 249 (v)
30. BD ( 1) C 14 - C 15	1.97858	-0.66279 426 (v) , 432 (v) , 431 (g) , 429 (g) 276 (v) , 234 (v)
31. BD ( 2) C 14 - C 15	1.90232	-0.24531 423 (v)
32. BD ( 1) C 14 - H 21	1.98166	-0.50080 422 (v) , 430 (v) , 263 (v) , 234 (v) 427 (g) , 235 (v)
33. BD ( 1) C 15 - N 16	1.98310	-0.72828 429 (v) , 421 (v) , 220 (v) , 424 (g) 422 (v) , 426 (r) , 306 (v) , 427 (g) 438 (v) , 222 (v)
34. BD ( 1) C 15 - H 22	1.98163	-0.50112 424 (v) , 425 (v) , 276 (v) , 249 (v) 427 (g)
35. BD ( 1) N 16 - C 18	1.99096	-0.70524 422 (v) , 427 (v) , 424 (g) , 263 (v) 220 (v)
36. BD ( 1) C 17 - H 23	1.98684	-0.45947 422 (v) , 236 (v)
37. BD ( 1) C 17 - H 24	1.98534	-0.45284 423 (v) , 425 (v)
38. BD ( 1) C 17 - H 25	1.98070	-0.44547 425 (v) , 423 (v) , 64 (r)
39. BD ( 1) C 18 - H 26	1.98702	-0.46776 424 (v)
40. BD ( 1) C 18 - H 27	1.98581	-0.46173 424 (v)
41. BD ( 1) C 18 - H 28	1.98196	-0.45924 430 (v) , 64 (r) , 278 (v)
42. CR ( 1) N 1	1.99944	-13.87384 83 (v) , 124 (v) , 194 (v) , 403 (v)
43. CR ( 1) C 2	1.99879	-9.79530 403 (g) , 411 (v) , 405 (v) , 400 (v) 137 (v) , 410 (v) , 399 (v) , 404 (v)
44. CR ( 1) N 3	1.99944	-13.87238 110 (v) , 83 (v) , 403 (v) , 180 (v)
45. CR ( 1) C 4	1.99912	-9.79279 123 (v) , 405 (v) , 406 (g) , 409 (v) 96 (v) , 401 (v)
46. CR ( 1) C 5	1.99911	-9.79369 109 (v) , 400 (v) , 406 (g) , 408 (v) 398 (v) , 68 (v)
47. CR ( 1) B 6	1.99710	-6.29852 421 (v) , 412 (v) , 206 (v) , 411 (g) 398 (v) , 401 (v) , 150 (v) , 414 (v) 80 (v) , 410 (g) , 153 (v)
48. CR ( 1) C 7	1.99861	-9.72898 403 (v) , 410 (g) , 412 (g) , 421 (v) 414 (g) , 167 (v) , 61 (v) , 206 (v)
49. CR ( 1) O 8	1.99982	-18.39812 150 (v) , 410 (v) , 414 (v)
50. CR ( 1) C 9	1.99931	-9.78472 401 (v) , 404 (v) , 405 (g)
51. CR ( 1) C 10	1.99933	-9.79479 399 (v) , 398 (v) , 400 (g)
52. CR ( 1) B 11	1.99777	-6.30929 403 (v) , 412 (v) , 424 (v) , 411 (g) 422 (v) , 410 (v) , 136 (v) , 220 (v) 61 (v) , 414 (g) , 150 (v)
53. CR ( 1) C 12	1.99873	-9.78013 421 (g) , 411 (v) , 206 (v) , 432 (v) 426 (v) , 210 (v) , 425 (v) , 430 (v)
54. CR ( 1) N 13	1.99946	-13.85352 250 (v) , 224 (v) , 292 (v) , 421 (v)
55. CR ( 1) C 14	1.99911	-9.77599 263 (v) , 426 (v) , 427 (g) , 431 (v) 422 (v) , 236 (v)
56. CR ( 1) C 15	1.99911	-9.77539 249 (v) , 432 (v) , 427 (g) , 429 (v) 278 (v) , 424 (v)
57. CR ( 1) N 16	1.99946	-13.85604 264 (v) , 222 (v) , 306 (v) , 421 (v)
58. CR ( 1) C 17	1.99933	-9.77888 425 (v) , 422 (v) , 426 (g)
59. CR ( 1) C 18	1.99934	-9.78819 424 (v) , 430 (v) , 432 (g)
60. LP ( 1) N 1	1.52100	-0.24336 402 (v) , 407 (v) , 420 (v) , 418 (v) 122 (v) , 192 (v) , 85 (v)
61. LP ( 1) B 6	0.74739	0.03098 64 (v) , 413 (v) , 402 (v) , 410 (g)

62. LP (	1) O	8	1.96911	411 (g), 151 (v), 86 (v), 140 (g)
63. LP (	2) O	8	1.77279	-0.56215 150 (v), 410 (v), 414 (v), 156 (v)
64. LP* (	1) B	11	0.61730	-0.14586 414 (v), 410 (v), 152 (v), 154 (v)
				0.02666 61 (v), 413 (v), 423 (v), 424 (v)
				422 (v), 402 (r)
65. LP (	1) N	16	1.55922	-0.22363 423 (v), 428 (v), 437 (v), 262 (v)
				436 (v), 304 (v), 225 (v), 438 (v)
66. RY* (	1) N	1	0.00407	1.64929
67. RY* (	2) N	1	0.00243	0.56668
68. RY* (	3) N	1	0.00202	1.30632
69. RY* (	4) N	1	0.00084	1.02597
70. RY* (	5) N	1	0.00063	2.21781
71. RY* (	6) N	1	0.00040	2.19843
72. RY* (	7) N	1	0.00019	2.61945
73. RY* (	8) N	1	0.00015	2.40983
74. RY* (	9) N	1	0.00013	2.55384
75. RY* (	10) N	1	0.00006	3.17706
76. RY* (	11) N	1	0.00003	2.49678
77. RY* (	12) N	1	0.00002	2.85298
78. RY* (	13) N	1	0.00000	2.09040
79. RY* (	14) N	1	0.00000	29.71668
80. RY* (	1) C	2	0.00504	1.79746
81. RY* (	2) C	2	0.00255	1.12426
82. RY* (	3) C	2	0.00211	1.39063
83. RY* (	4) C	2	0.00192	1.24079
84. RY* (	5) C	2	0.00113	1.76648
85. RY* (	6) C	2	0.00107	1.66004
86. RY* (	7) C	2	0.00042	1.44685
87. RY* (	8) C	2	0.00022	1.59384
88. RY* (	9) C	2	0.00017	1.87807
89. RY* (	10) C	2	0.00012	2.14347
90. RY* (	11) C	2	0.00007	1.82798
91. RY* (	12) C	2	0.00005	1.36688
92. RY* (	13) C	2	0.00002	2.70448
93. RY* (	14) C	2	0.00000	20.74422
94. RY* (	1) N	3	0.00403	1.64630
95. RY* (	2) N	3	0.00236	0.57485
96. RY* (	3) N	3	0.00199	1.23282
97. RY* (	4) N	3	0.00079	1.14459
98. RY* (	5) N	3	0.00069	2.21221
99. RY* (	6) N	3	0.00041	2.19645
100. RY* (	7) N	3	0.00020	2.43351
101. RY* (	8) N	3	0.00014	2.57605
102. RY* (	9) N	3	0.00015	2.75679
103. RY* (	10) N	3	0.00008	2.88025
104. RY* (	11) N	3	0.00003	2.54576
105. RY* (	12) N	3	0.00002	2.80322
106. RY* (	13) N	3	0.00000	2.08211
107. RY* (	14) N	3	0.00000	29.77824
108. RY* (	1) C	4	0.00384	0.55393
109. RY* (	2) C	4	0.00300	1.40013
110. RY* (	3) C	4	0.00127	1.25421
111. RY* (	4) C	4	0.00050	0.93975
112. RY* (	5) C	4	0.00042	1.74204
113. RY* (	6) C	4	0.00015	1.61242
114. RY* (	7) C	4	0.00012	1.81340
115. RY* (	8) C	4	0.00008	1.83144
116. RY* (	9) C	4	0.00005	2.21585
117. RY* (	10) C	4	0.00003	1.31004
118. RY* (	11) C	4	0.00002	1.52528
119. RY* (	12) C	4	0.00000	20.95521
120. RY* (	13) C	4	0.00000	1.76082
121. RY* (	14) C	4	0.00001	2.02630
122. RY* (	1) C	5	0.00382	0.54967
123. RY* (	2) C	5	0.00294	1.40571
124. RY* (	3) C	5	0.00131	1.24954
125. RY* (	4) C	5	0.00051	0.87913
126. RY* (	5) C	5	0.00042	1.74661
127. RY* (	6) C	5	0.00015	1.72437
128. RY* (	7) C	5	0.00012	1.81321
129. RY* (	8) C	5	0.00008	1.69970

130.	RY*	( 9)	C	5	0.00005	2.10429
131.	RY*	( 10)	C	5	0.00002	1.30625
132.	RY*	( 11)	C	5	0.00003	1.93792
133.	RY*	( 12)	C	5	0.00000	1.77597
134.	RY*	( 13)	C	5	0.00001	1.81758
135.	RY*	( 14)	C	5	0.00000	20.89909
136.	RY*	( 1)	B	6	0.00332	2.00685
137.	RY*	( 2)	B	6	0.00186	1.35358
138.	RY*	( 3)	B	6	0.00121	1.20245
139.	RY*	( 4)	B	6	0.00078	0.99643
140.	RY*	( 5)	B	6	0.00065	0.98695
141.	RY*	( 6)	B	6	0.00052	0.75510
142.	RY*	( 7)	B	6	0.00029	2.75707
143.	RY*	( 8)	B	6	0.00027	2.23249
144.	RY*	( 9)	B	6	0.00015	1.34008
145.	RY*	( 10)	B	6	0.00012	0.91363
146.	RY*	( 11)	B	6	0.00008	2.07566
147.	RY*	( 12)	B	6	0.00004	1.46117
148.	RY*	( 13)	B	6	0.00005	11.14555
149.	RY*	( 14)	B	6	0.00004	1.74950
150.	RY*	( 1)	C	7	0.01708	0.84863
151.	RY*	( 2)	C	7	0.00511	1.92254
152.	RY*	( 3)	C	7	0.00299	2.24312
153.	RY*	( 4)	C	7	0.00136	1.85147
154.	RY*	( 5)	C	7	0.00024	1.33903
155.	RY*	( 6)	C	7	0.00022	2.43278
156.	RY*	( 7)	C	7	0.00013	1.42155
157.	RY*	( 8)	C	7	0.00009	1.02950
158.	RY*	( 9)	C	7	0.00006	1.30615
159.	RY*	( 10)	C	7	0.00006	1.27758
160.	RY*	( 11)	C	7	0.00004	1.21689
161.	RY*	( 12)	C	7	0.00000	21.46799
162.	RY*	( 13)	C	7	0.00001	1.71676
163.	RY*	( 14)	C	7	0.00001	1.98064
164.	RY*	( 1)	O	8	0.00547	0.76907
165.	RY*	( 2)	O	8	0.00304	0.67966
166.	RY*	( 3)	O	8	0.00190	1.10687
167.	RY*	( 4)	O	8	0.00029	1.21061
168.	RY*	( 5)	O	8	0.00005	4.14633
169.	RY*	( 6)	O	8	0.00000	41.36157
170.	RY*	( 7)	O	8	0.00001	2.99388
171.	RY*	( 8)	O	8	0.00001	2.75984
172.	RY*	( 9)	O	8	0.00000	2.65991
173.	RY*	( 10)	O	8	0.00000	2.87170
174.	RY*	( 11)	O	8	0.00000	2.66025
175.	RY*	( 12)	O	8	0.00000	2.83597
176.	RY*	( 13)	O	8	0.00001	3.69880
177.	RY*	( 14)	O	8	0.00000	2.74371
178.	RY*	( 1)	C	9	0.00172	0.82628
179.	RY*	( 2)	C	9	0.00162	0.85087
180.	RY*	( 3)	C	9	0.00121	0.83265
181.	RY*	( 4)	C	9	0.00034	1.33638
182.	RY*	( 5)	C	9	0.00012	1.56057
183.	RY*	( 6)	C	9	0.00006	0.97363
184.	RY*	( 7)	C	9	0.00005	1.43791
185.	RY*	( 8)	C	9	0.00005	1.68654
186.	RY*	( 9)	C	9	0.00003	2.39549
187.	RY*	( 10)	C	9	0.00001	2.38194
188.	RY*	( 11)	C	9	0.00002	1.99671
189.	RY*	( 12)	C	9	0.00001	2.25296
190.	RY*	( 13)	C	9	0.00000	20.91094
191.	RY*	( 14)	C	9	0.00000	2.13759
192.	RY*	( 1)	C	10	0.00214	0.70662
193.	RY*	( 2)	C	10	0.00162	0.82370
194.	RY*	( 3)	C	10	0.00081	1.25134
195.	RY*	( 4)	C	10	0.00022	1.37552
196.	RY*	( 5)	C	10	0.00013	1.75034
197.	RY*	( 6)	C	10	0.00009	1.11246
198.	RY*	( 7)	C	10	0.00005	1.39404
199.	RY*	( 8)	C	10	0.00003	1.94742
200.	RY*	( 9)	C	10	0.00003	1.52866

201.	RY*	( 10)	C	10	0.00001	2.29970
202.	RY*	( 11)	C	10	0.00002	2.22291
203.	RY*	( 12)	C	10	0.00001	2.13343
204.	RY*	( 13)	C	10	0.00000	20.60421
205.	RY*	( 14)	C	10	0.00000	2.15014
206.	RY*	( 1)	B	11	0.00346	1.24933
207.	RY*	( 2)	B	11	0.00204	1.40178
208.	RY*	( 3)	B	11	0.00147	1.77009
209.	RY*	( 4)	B	11	0.00103	1.01301
210.	RY*	( 5)	B	11	0.00075	1.15957
211.	RY*	( 6)	B	11	0.00049	1.10514
212.	RY*	( 7)	B	11	0.00035	2.22874
213.	RY*	( 8)	B	11	0.00024	1.42871
214.	RY*	( 9)	B	11	0.00016	1.52018
215.	RY*	( 10)	B	11	0.00012	1.34058
216.	RY*	( 11)	B	11	0.00009	1.55769
217.	RY*	( 12)	B	11	0.00007	6.35779
218.	RY*	( 13)	B	11	0.00004	1.62229
219.	RY*	( 14)	B	11	0.00004	1.72453
220.	RY*	( 1)	C	12	0.00478	1.80412
221.	RY*	( 2)	C	12	0.00303	1.37477
222.	RY*	( 3)	C	12	0.00209	1.16608
223.	RY*	( 4)	C	12	0.00185	1.37102
224.	RY*	( 5)	C	12	0.00146	1.61984
225.	RY*	( 6)	C	12	0.00092	1.76470
226.	RY*	( 7)	C	12	0.00056	1.17684
227.	RY*	( 8)	C	12	0.00045	1.38499
228.	RY*	( 9)	C	12	0.00016	1.91741
229.	RY*	( 10)	C	12	0.00008	1.89591
230.	RY*	( 11)	C	12	0.00007	2.33622
231.	RY*	( 12)	C	12	0.00005	1.72212
232.	RY*	( 13)	C	12	0.00003	2.62996
233.	RY*	( 14)	C	12	0.00000	20.83947
234.	RY*	( 1)	N	13	0.00409	1.26562
235.	RY*	( 2)	N	13	0.00366	1.10446
236.	RY*	( 3)	N	13	0.00184	1.26264
237.	RY*	( 4)	N	13	0.00084	1.18658
238.	RY*	( 5)	N	13	0.00061	2.19443
239.	RY*	( 6)	N	13	0.00045	2.24146
240.	RY*	( 7)	N	13	0.00021	2.58338
241.	RY*	( 8)	N	13	0.00013	2.49095
242.	RY*	( 9)	N	13	0.00011	2.40005
243.	RY*	( 10)	N	13	0.00009	3.07406
244.	RY*	( 11)	N	13	0.00005	2.52641
245.	RY*	( 12)	N	13	0.00002	2.80832
246.	RY*	( 13)	N	13	0.00001	2.11231
247.	RY*	( 14)	N	13	0.00000	29.79893
248.	RY*	( 1)	C	14	0.00396	0.65050
249.	RY*	( 2)	C	14	0.00302	1.34246
250.	RY*	( 3)	C	14	0.00133	1.26359
251.	RY*	( 4)	C	14	0.00055	1.00965
252.	RY*	( 5)	C	14	0.00046	1.69440
253.	RY*	( 6)	C	14	0.00015	1.57713
254.	RY*	( 7)	C	14	0.00013	1.71853
255.	RY*	( 8)	C	14	0.00007	2.04479
256.	RY*	( 9)	C	14	0.00005	2.17191
257.	RY*	( 10)	C	14	0.00003	1.45450
258.	RY*	( 11)	C	14	0.00003	1.56086
259.	RY*	( 12)	C	14	0.00001	1.66346
260.	RY*	( 13)	C	14	0.00001	2.01661
261.	RY*	( 14)	C	14	0.00000	20.96601
262.	RY*	( 1)	C	15	0.00456	0.53712
263.	RY*	( 2)	C	15	0.00292	1.40051
264.	RY*	( 3)	C	15	0.00130	1.26105
265.	RY*	( 4)	C	15	0.00054	0.94485
266.	RY*	( 5)	C	15	0.00044	1.75752
267.	RY*	( 6)	C	15	0.00017	1.63391
268.	RY*	( 7)	C	15	0.00012	1.79374
269.	RY*	( 8)	C	15	0.00005	2.07183
270.	RY*	( 9)	C	15	0.00006	1.87571
271.	RY*	( 10)	C	15	0.00002	1.50944

272.	RY*	( 11)	C	15	0.00002	2.02528
273.	RY*	( 12)	C	15	0.00001	1.73792
274.	RY*	( 13)	C	15	0.00000	1.77368
275.	RY*	( 14)	C	15	0.00000	20.78882
276.	RY*	( 1)	N	16	0.00393	1.55927
277.	RY*	( 2)	N	16	0.00325	0.74900
278.	RY*	( 3)	N	16	0.00201	1.30824
279.	RY*	( 4)	N	16	0.00068	1.82088
280.	RY*	( 5)	N	16	0.00054	1.51716
281.	RY*	( 6)	N	16	0.00042	2.22885
282.	RY*	( 7)	N	16	0.00017	2.52349
283.	RY*	( 8)	N	16	0.00013	2.46056
284.	RY*	( 9)	N	16	0.00012	2.45477
285.	RY*	( 10)	N	16	0.00008	2.98729
286.	RY*	( 11)	N	16	0.00005	2.55291
287.	RY*	( 12)	N	16	0.00001	2.18240
288.	RY*	( 13)	N	16	0.00002	2.83930
289.	RY*	( 14)	N	16	0.00000	29.74431
290.	RY*	( 1)	C	17	0.00170	0.84177
291.	RY*	( 2)	C	17	0.00162	0.90151
292.	RY*	( 3)	C	17	0.00084	1.24001
293.	RY*	( 4)	C	17	0.00024	1.33834
294.	RY*	( 5)	C	17	0.00014	1.57138
295.	RY*	( 6)	C	17	0.00009	1.51980
296.	RY*	( 7)	C	17	0.00006	1.47605
297.	RY*	( 8)	C	17	0.00004	1.41988
298.	RY*	( 9)	C	17	0.00003	2.09880
299.	RY*	( 10)	C	17	0.00001	2.50761
300.	RY*	( 11)	C	17	0.00002	2.19393
301.	RY*	( 12)	C	17	0.00000	20.45710
302.	RY*	( 13)	C	17	0.00001	1.92977
303.	RY*	( 14)	C	17	0.00001	2.11711
304.	RY*	( 1)	C	18	0.00206	0.83931
305.	RY*	( 2)	C	18	0.00169	0.83538
306.	RY*	( 3)	C	18	0.00084	1.21776
307.	RY*	( 4)	C	18	0.00018	1.43215
308.	RY*	( 5)	C	18	0.00011	1.71478
309.	RY*	( 6)	C	18	0.00007	1.56861
310.	RY*	( 7)	C	18	0.00005	2.00143
311.	RY*	( 8)	C	18	0.00003	1.21352
312.	RY*	( 9)	C	18	0.00001	1.37233
313.	RY*	( 10)	C	18	0.00002	2.25405
314.	RY*	( 11)	C	18	0.00001	2.09608
315.	RY*	( 12)	C	18	0.00002	2.21009
316.	RY*	( 13)	C	18	0.00001	2.37511
317.	RY*	( 14)	C	18	0.00000	20.26996
318.	RY*	( 1)	H	19	0.00033	1.43499
319.	RY*	( 2)	H	19	0.00027	1.57252
320.	RY*	( 3)	H	19	0.00017	1.19725
321.	RY*	( 4)	H	19	0.00015	1.58046
322.	RY*	( 5)	H	19	0.00004	2.70293
323.	RY*	( 1)	H	20	0.00047	0.90161
324.	RY*	( 2)	H	20	0.00028	1.57081
325.	RY*	( 3)	H	20	0.00020	1.41462
326.	RY*	( 4)	H	20	0.00016	1.88198
327.	RY*	( 5)	H	20	0.00004	2.70516
328.	RY*	( 1)	H	21	0.00036	1.29365
329.	RY*	( 2)	H	21	0.00029	1.58639
330.	RY*	( 3)	H	21	0.00017	1.02828
331.	RY*	( 4)	H	21	0.00016	1.91934
332.	RY*	( 5)	H	21	0.00004	2.73023
333.	RY*	( 1)	H	22	0.00034	1.39619
334.	RY*	( 2)	H	22	0.00030	1.58634
335.	RY*	( 3)	H	22	0.00017	1.04641
336.	RY*	( 4)	H	22	0.00016	1.78487
337.	RY*	( 5)	H	22	0.00004	2.72857
338.	RY*	( 1)	H	23	0.00051	0.91015
339.	RY*	( 2)	H	23	0.00021	1.28788
340.	RY*	( 3)	H	23	0.00014	1.74573
341.	RY*	( 4)	H	23	0.00010	1.93348
342.	RY*	( 5)	H	23	0.00002	2.66991

343.	RY*	( 1)	H	24	0.00139	0.75992	
344.	RY*	( 2)	H	24	0.00020	1.68188	
345.	RY*	( 3)	H	24	0.00015	1.70321	
346.	RY*	( 4)	H	24	0.00009	1.87121	
347.	RY*	( 5)	H	24	0.00003	2.62228	
348.	RY*	( 1)	H	25	0.00187	0.80390	
349.	RY*	( 2)	H	25	0.00028	1.78002	
350.	RY*	( 3)	H	25	0.00016	1.81033	
351.	RY*	( 4)	H	25	0.00010	1.83162	
352.	RY*	( 5)	H	25	0.00004	2.65759	
353.	RY*	( 1)	H	26	0.00084	0.75634	
354.	RY*	( 2)	H	26	0.00023	1.41696	
355.	RY*	( 3)	H	26	0.00014	1.76531	
356.	RY*	( 4)	H	26	0.00009	1.91432	
357.	RY*	( 5)	H	26	0.00002	2.62701	
358.	RY*	( 1)	H	27	0.00137	0.77807	
359.	RY*	( 2)	H	27	0.00017	1.49376	
360.	RY*	( 3)	H	27	0.00014	1.75223	
361.	RY*	( 4)	H	27	0.00009	1.91613	
362.	RY*	( 5)	H	27	0.00003	2.61942	
363.	RY*	( 1)	H	28	0.00079	1.08141	
364.	RY*	( 2)	H	28	0.00024	1.79000	
365.	RY*	( 3)	H	28	0.00018	1.66820	
366.	RY*	( 4)	H	28	0.00008	1.64744	
367.	RY*	( 5)	H	28	0.00003	2.71755	
368.	RY*	( 1)	H	29	0.00080	0.88355	
369.	RY*	( 2)	H	29	0.00018	1.26642	
370.	RY*	( 3)	H	29	0.00015	1.78002	
371.	RY*	( 4)	H	29	0.00009	1.93692	
372.	RY*	( 5)	H	29	0.00003	2.60006	
373.	RY*	( 1)	H	30	0.00071	1.15240	
374.	RY*	( 2)	H	30	0.00028	1.89983	
375.	RY*	( 3)	H	30	0.00011	1.55773	
376.	RY*	( 4)	H	30	0.00010	1.74649	
377.	RY*	( 5)	H	30	0.00003	2.77632	
378.	RY*	( 1)	H	31	0.00090	0.84810	
379.	RY*	( 2)	H	31	0.00018	1.29409	
380.	RY*	( 3)	H	31	0.00014	1.78208	
381.	RY*	( 4)	H	31	0.00009	1.93144	
382.	RY*	( 5)	H	31	0.00003	2.61144	
383.	RY*	( 1)	H	32	0.00067	0.98516	
384.	RY*	( 2)	H	32	0.00019	1.23750	
385.	RY*	( 3)	H	32	0.00015	1.73625	
386.	RY*	( 4)	H	32	0.00009	1.96606	
387.	RY*	( 5)	H	32	0.00003	2.60505	
388.	RY*	( 1)	H	33	0.00074	0.97777	
389.	RY*	( 2)	H	33	0.00018	1.24894	
390.	RY*	( 3)	H	33	0.00014	1.74368	
391.	RY*	( 4)	H	33	0.00009	1.96738	
392.	RY*	( 5)	H	33	0.00003	2.60096	
393.	RY*	( 1)	H	34	0.00217	0.88438	
394.	RY*	( 2)	H	34	0.00035	1.98983	
395.	RY*	( 3)	H	34	0.00012	1.84695	
396.	RY*	( 4)	H	34	0.00010	1.76315	
397.	RY*	( 5)	H	34	0.00004	2.57905	
398.	BD*	( 1)	N	1 - C	2	0.04797	0.36301
399.	BD*	( 1)	N	1 - C	5	0.02785	0.33968
400.	BD*	( 1)	N	1 - C	10	0.01663	0.24388
401.	BD*	( 1)	C	2 - N	3	0.04502	0.36528
402.	BD*	( 2)	C	2 - N	3	0.58815	-0.04941 407 (v) , 61 (v) , 81 (g) , 416 (v) 95 (g) , 98 (g) , 415 (v) , 64 (r) 108 (v)
403.	BD*	( 1)	C	2 - B	6	0.05872	0.41973
404.	BD*	( 1)	N	3 - C	4	0.02694	0.34219
405.	BD*	( 1)	N	3 - C	9	0.01793	0.24509
406.	BD*	( 1)	C	4 - C	5	0.00852	0.46216
407.	BD*	( 2)	C	4 - C	5	0.29507	-0.03722 402 (v) , 126 (g) , 112 (g)
408.	BD*	( 1)	C	4 - H	19	0.01201	0.30357
409.	BD*	( 1)	C	5 - H	20	0.01274	0.30162
410.	BD*	( 1)	B	6 - C	7	0.07253	0.45666
411.	BD*	( 1)	B	6 - B	11	0.03873	0.49860



412.	BD*	( 1)	C	7 - O	8	0.04637	0.53003	
413.	BD*	( 2)	C	7 - O	8	0.43205	0.05820	61 (v), 64 (v), 165 (g), 151 (g)
								412 (g), 160 (g)
414.	BD*	( 1)	C	7 - B	11	0.11509	0.35456	424 (v), 422 (v), 417 (r), 411 (g)
								419 (r), 398 (r), 430 (r), 152 (g)
								412 (g), 423 (v), 438 (r), 210 (g)
								208 (g)
415.	BD*	( 1)	C	9 - H	32	0.01137	0.28970	
416.	BD*	( 1)	C	9 - H	33	0.01225	0.28954	
417.	BD*	( 1)	C	9 - H	34	0.00878	0.33768	
418.	BD*	( 1)	C	10 - H	29	0.01206	0.28012	
419.	BD*	( 1)	C	10 - H	30	0.01214	0.31327	
420.	BD*	( 1)	C	10 - H	31	0.01312	0.27901	
421.	BD*	( 1)	B	11 - C	12	0.03334	0.44445	
422.	BD*	( 1)	C	12 - N	13	0.04275	0.36586	
423.	BD*	( 2)	C	12 - N	13	0.69287	-0.03532	428 (v), 64 (v), 414 (v), 221 (g)
								434 (v), 411 (v), 223 (g), 238 (g)
								435 (v), 248 (v)
424.	BD*	( 1)	C	12 - N	16	0.04534	0.36067	
425.	BD*	( 1)	N	13 - C	14	0.02556	0.35692	
426.	BD*	( 1)	N	13 - C	17	0.01595	0.26504	
427.	BD*	( 1)	C	14 - C	15	0.00849	0.48394	
428.	BD*	( 2)	C	14 - C	15	0.30224	-0.01930	423 (v), 252 (g)
429.	BD*	( 1)	C	14 - H	21	0.01215	0.31953	
430.	BD*	( 1)	C	15 - N	16	0.02647	0.35008	
431.	BD*	( 1)	C	15 - H	22	0.01206	0.31863	
432.	BD*	( 1)	N	16 - C	18	0.01628	0.26332	
433.	BD*	( 1)	C	17 - H	23	0.00663	0.29938	
434.	BD*	( 1)	C	17 - H	24	0.01955	0.29774	
435.	BD*	( 1)	C	17 - H	25	0.01126	0.32647	
436.	BD*	( 1)	C	18 - H	26	0.01138	0.28819	
437.	BD*	( 1)	C	18 - H	27	0.01881	0.29100	
438.	BD*	( 1)	C	18 - H	28	0.01221	0.30536	
-----								
	Total Lewis			123.92151	( 96.8137%)			
	Valence non-Lewis			3.86264	( 3.0177%)			
	Rydberg non-Lewis			0.21585	( 0.1686%)			
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	Total unit 1			128.00000	(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:	49	42	44	57	54	43	51	46	45	59
Sorting of NBOs:	50	53	58	55	56	48	52	47	15	1
Sorting of NBOs:	2	4	7	28	33	27	25	3	35	8
Sorting of NBOs:	29	9	30	62	12	11	24	6	34	32
Sorting of NBOs:	21	23	39	22	18	19	40	36	41	37
Sorting of NBOs:	20	38	13	17	5	26	14	10	16	31
Sorting of NBOs:	60	65	63	402	407	423	428	64	61	413
Sorting of NBOs:	400	405	432	426	420	418	436	416	415	437
Sorting of NBOs:	434	433	409	408	438	419	431	429	435	417
Sorting of NBOs:	399	404	430	414	425	424	398	401	422	403
Sorting of NBOs:	421	410	406	427	411	412	262	122	108	67
Sorting of NBOs:	95	248	165	192	277	141	353	343	164	358
Sorting of NBOs:	348	193	178	180	305	304	290	378	150	179
Sorting of NBOs:	125	368	393	291	323	338	145	111	265	183
Sorting of NBOs:	388	383	140	139	251	209	69	330	157	335
Sorting of NBOs:	363	235	211	166	197	81	97	373	210	222
Sorting of NBOs:	226	237	320	138	167	311	160	306	96	384
Sorting of NBOs:	292	83	389	206	124	194	110	264	236	250
Sorting of NBOs:	234	369	159	339	328	379	158	131	68	278
Sorting of NBOs:	117	181	293	154	144	215	249	137	91	223
Sorting of NBOs:	312	221	195	227	82	198	333	109	263	207
Sorting of NBOs:	123	325	354	297	156	213	307	318	184	86
Sorting of NBOs:	257	147	296	359	271	280	295	214	118	200
Sorting of NBOs:	216	375	276	182	258	309	324	294	319	253
Sorting of NBOs:	321	334	329	87	113	224	218	267	94	366



Labels of output orbitals: BD\*  
BD\* BD\* BD\*  
Labels of output orbitals: BD\* BD\* BD\* BD\* BD\* BD\* 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\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*  
Labels of output orbitals: RY\*  
RY\* RY\* RY\*

```
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,-7.158933\H,0,-1.023842,-5.33392,-7.676287\H,0,-5.129739,-3.173636,-6
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```

THERE IS MUCH PLEASURE TO BE GAINED FROM USELESS KNOWLEDGE

-- BERTRAND RUSSELL

```
Job cpu time: 0 days 1 hours 26 minutes 51.1 seconds.
File lengths (MBytes): RWF= 109 Int= 0 D2E= 0 Chk= 8 Scr= 1
Normal termination of Gaussian 09 at Wed Oct 28 23:45:56 2015.
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