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Tables of optimized geometries:

1 Triplet UHF/6-31G*:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	-1.024853
2	6	0.000000	0.000000	1.784015
3	6	0.000000	1.244951	-0.336515
4	6	0.000000	-1.244951	-0.336515
5	6	0.000000	1.214943	1.095060
6	6	0.000000	-1.214943	1.095060
7	6	0.000000	2.462384	-1.036459
8	6	0.000000	-2.462384	-1.036459
9	1	0.000000	0.000000	-2.101073
10	1	0.000000	0.000000	2.859584
11	1	0.000000	2.142988	1.638596
12	1	0.000000	-2.142988	1.638596
13	1	0.000000	2.487421	-2.110656
14	1	0.000000	-2.487421	-2.110656
15	1	0.000000	3.403079	-0.517198
16	1	0.000000	-3.403079	-0.517198

1 Singlet GVB(1/2)/6-31G*:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	-0.991976
2	6	0.000000	0.000000	1.766588
3	6	0.000000	1.217202	-0.314323
4	6	0.000000	-1.217202	-0.314323
5	6	0.000000	1.201520	1.080789
6	6	0.000000	-1.201520	1.080789
7	6	0.000000	2.477650	-1.047627
8	6	0.000000	-2.477650	-1.047627
9	1	0.000000	0.000000	-2.068579
10	1	0.000000	0.000000	2.842275
11	1	0.000000	2.130278	1.623757
12	1	0.000000	-2.130278	1.623757
13	1	0.000000	2.490451	-2.119811
14	1	0.000000	-2.490451	-2.119811
15	1	0.000000	3.415402	-0.527672
16	1	0.000000	-3.415402	-0.527672

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3 Triplet UHF/6-31G:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.000000	0.000000	1.016981
2	6	0.000000	0.000000	-1.800484
3	6	0.000000	1.189795	0.334672
4	6	0.000000	-1.189795	0.334672
5	6	0.000000	1.206784	-1.095251
6	6	0.000000	-1.206784	-1.095251
7	6	0.000000	2.363436	1.105272
8	6	0.000000	-2.363436	1.105272
9	1	0.000000	0.000000	-2.873231
10	1	0.000000	2.147304	-1.610784
11	1	0.000000	-2.147304	-1.610784
12	1	0.000000	2.293451	2.173622
13	1	0.000000	-2.293451	2.173622
14	1	0.000000	3.333737	0.647637
15	1	0.000000	-3.333737	0.647637

3 Singlet GVB(1/2)/6-31G:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.000000	0.000000	0.981503
2	6	0.000000	0.000000	-1.775908
3	6	0.000000	1.161167	0.317384
4	6	0.000000	-1.161167	0.317384
5	6	0.000000	1.195597	-1.077744
6	6	0.000000	-1.195597	-1.077744
7	6	0.000000	2.380390	1.109228
8	6	0.000000	-2.380390	1.109228
9	1	0.000000	0.000000	-2.848776
10	1	0.000000	2.135107	-1.593441
11	1	0.000000	-2.135107	-1.593441
12	1	0.000000	2.306088	2.175638
13	1	0.000000	-2.306088	2.175638
14	1	0.000000	3.343914	0.641448
15	1	0.000000	-3.343914	0.641448

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4 Triplet UHF/6-31G*:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	-1.061560
2	7	0.000000	0.000000	1.667277
3	6	0.000000	1.241048	-0.369391
4	6	0.000000	-1.241048	-0.369391
5	6	0.000000	1.186091	1.047439
6	6	0.000000	-1.186091	1.047439
7	6	0.000000	2.487868	-1.018315
8	6	0.000000	-2.487868	-1.018315
9	1	0.000000	0.000000	-2.135220
10	1	0.000000	0.000000	2.671504
11	1	0.000000	2.055120	1.674040
12	1	0.000000	-2.055120	1.674040
13	1	0.000000	2.548270	-2.089240
14	1	0.000000	-2.548270	-2.089240
15	1	0.000000	3.405810	-0.462132
16	1	0.000000	-3.405810	-0.462132

4 Singlet GVB(1/2)/6-31G*:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	-1.011368
2	7	0.000000	0.000000	1.667715
3	6	0.000000	1.224935	-0.339176
4	6	0.000000	-1.224935	-0.339176
5	6	0.000000	1.178175	1.044822
6	6	0.000000	-1.178175	1.044822
7	6	0.000000	2.487346	-1.056477
8	6	0.000000	-2.487346	-1.056477
9	1	0.000000	0.000000	-2.086202
10	1	0.000000	0.000000	2.669597
11	1	0.000000	2.051456	1.665645
12	1	0.000000	-2.051456	1.665645
13	1	0.000000	2.499547	-2.127082
14	1	0.000000	-2.499547	-2.127082
15	1	0.000000	3.419165	-0.528176
16	1	0.000000	-3.419165	-0.528176

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5 Triplet UHF/6-31G*:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.052778	0.000000
2	6	0.033042	-1.714429	0.000000
3	6	-1.211335	0.333056	0.000000
4	6	1.255326	0.388665	0.000000
5	7	-1.112531	-1.043307	0.000000
6	6	1.240920	-1.033943	0.000000
7	6	-2.493238	0.898511	0.000000
8	6	2.470876	1.096406	0.000000
9	1	-0.046716	2.124424	0.000000
10	1	-0.035440	-2.784282	0.000000
11	1	-1.966364	-1.570204	0.000000
12	1	2.153701	-1.597182	0.000000
13	1	-2.608310	1.963852	0.000000
14	1	2.485655	2.169303	0.000000
15	1	-3.379359	0.291856	0.000000
16	1	3.410997	0.579122	0.000000

5 Singlet GVB(1/2)/6-31G*:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.017547	0.000000
2	6	0.054764	-1.723391	0.000000
3	6	-1.191117	0.302568	0.000000
4	6	1.229867	0.360629	0.000000
5	7	-1.124370	-1.049558	0.000000
6	6	1.230345	-1.069257	0.000000
7	6	-2.441159	0.970821	0.000000
8	6	2.421909	1.127153	0.000000
9	1	-0.044328	2.089209	0.000000
10	1	-0.019627	-2.792495	0.000000
11	1	-1.973511	-1.574627	0.000000
12	1	2.151799	-1.616774	0.000000
13	1	-2.470360	2.040814	0.000000
14	1	2.383716	2.198433	0.000000
15	1	-3.368754	0.432128	0.000000
16	1	3.384010	0.653801	0.000000

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6 Triplet UHF/6-31G*:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.000000	0.000000	0.911967
2	6	0.000000	0.000000	-1.818389
3	6	0.000000	1.210361	0.292675
4	6	0.000000	-1.210361	0.292675
5	6	0.000000	1.208845	-1.127515
6	6	0.000000	-1.208845	-1.127515
7	6	0.000000	2.363365	1.097939
8	6	0.000000	-2.363365	1.097939
9	1	0.000000	0.000000	1.915883
10	1	0.000000	0.000000	-2.891708
11	1	0.000000	2.149942	-1.641165
12	1	0.000000	-2.149942	-1.641165
13	1	0.000000	2.303236	2.170173
14	1	0.000000	-2.303236	2.170173
15	1	0.000000	3.333923	0.643592
16	1	0.000000	-3.333923	0.643592

6 Singlet GVB(1/2)/6-31G*:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	0.000000	0.000000	0.934562
2	6	0.000000	0.000000	-1.778757
3	6	0.000000	1.203620	0.304034
4	6	0.000000	-1.203620	0.304034
5	6	0.000000	1.198851	-1.087334
6	6	0.000000	-1.198851	-1.087334
7	6	0.000000	2.408764	1.035415
8	6	0.000000	-2.408764	1.035415
9	1	0.000000	0.000000	1.934007
10	1	0.000000	0.000000	-2.852418
11	1	0.000000	2.135084	-1.610470
12	1	0.000000	-2.135084	-1.610470
13	1	0.000000	2.420730	2.107999
14	1	0.000000	-2.420730	2.107999
15	1	0.000000	3.343614	0.514285
16	1	0.000000	-3.343614	0.514285

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7 Triplet UHF/6-31G*:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	-1.075859
2	6	0.000000	0.000000	1.658541
3	6	0.000000	1.223989	-0.375187
4	6	0.000000	-1.223989	-0.375187
5	7	0.000000	1.141656	0.989971
6	7	0.000000	-1.141656	0.989971
7	6	0.000000	2.503380	-0.971538
8	6	0.000000	-2.503380	-0.971538
9	1	0.000000	0.000000	-2.148292
10	1	0.000000	0.000000	2.732716
11	1	0.000000	1.994298	1.531048
12	1	0.000000	-1.994298	1.531048
13	1	0.000000	2.592053	-2.040857
14	1	0.000000	-2.592053	-2.040857
15	1	0.000000	3.400420	-0.379897
16	1	0.000000	-3.400420	-0.379897

7 Singlet GVB(1/2)/6-31G*:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	-1.055643
2	6	0.000000	0.000000	1.681029
3	6	0.000000	1.217132	-0.370391
4	6	0.000000	-1.217132	-0.370391
5	7	0.000000	1.140221	1.041877
6	7	0.000000	-1.140221	1.041877
7	6	0.000000	2.411950	-1.034807
8	6	0.000000	-2.411950	-1.034807
9	1	0.000000	0.000000	-2.129649
10	1	0.000000	0.000000	2.755789
11	1	0.000000	1.986324	1.582229
12	1	0.000000	-1.986324	1.582229
13	1	0.000000	2.429257	-2.108584
14	1	0.000000	-2.429257	-2.108584
15	1	0.000000	3.359159	-0.524821
16	1	0.000000	-3.359159	-0.524821

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8 Triplet UHF/6-31G:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	-1.043484
2	6	0.000000	0.000000	1.806942
3	6	0.000000	1.236720	-0.308252
4	6	0.000000	-1.236720	-0.308252
5	6	0.000000	1.220698	1.123397
6	6	0.000000	-1.220698	1.123397
7	7	0.000000	2.385113	-0.967176
8	7	0.000000	-2.385113	-0.967176
9	1	0.000000	0.000000	-2.118110
10	1	0.000000	0.000000	2.878075
11	1	0.000000	2.146366	1.666407
12	1	0.000000	-2.146366	1.666407
13	1	0.000000	2.442324	-1.972102
14	1	0.000000	-2.442324	-1.972102
15	1	0.000000	3.270138	-0.485296
16	1	0.000000	-3.270138	-0.485296

8 1A1 Singlet GVB(1/2)/6-31G:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	-1.051714
2	6	0.000000	0.000000	1.823475
3	6	0.000000	1.195329	-0.351998
4	6	0.000000	-1.195329	-0.351998
5	6	0.000000	1.184660	1.115946
6	6	0.000000	-1.184660	1.115946
7	7	0.000000	2.387213	-0.938099
8	7	0.000000	-2.387213	-0.938099
9	1	0.000000	0.000000	-2.124360
10	1	0.000000	0.000000	2.894004
11	1	0.000000	2.121915	1.644714
12	1	0.000000	-2.121915	1.644714
13	1	0.000000	2.486344	-1.936691
14	1	0.000000	-2.486344	-1.936691
15	1	0.000000	3.248632	-0.425127
16	1	0.000000	-3.248632	-0.425127

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8 1B2 Singlet GVB(OSS)/6-31G:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.000000	-1.065938
2	6	0.000000	0.000000	1.790882
3	6	0.000000	1.268576	-0.316979
4	6	0.000000	-1.268576	-0.316979
5	6	0.000000	1.217010	1.132183
6	6	0.000000	-1.217010	1.132183
7	7	0.000000	2.389224	-0.954243
8	7	0.000000	-2.389224	-0.954243
9	1	0.000000	0.000000	-2.138928
10	1	0.000000	0.000000	2.863317
11	1	0.000000	2.137125	1.682632
12	1	0.000000	-2.137125	1.682632
13	1	0.000000	2.454123	-1.954746
14	1	0.000000	-2.454123	-1.954746
15	1	0.000000	3.271854	-0.476434
16	1	0.000000	-3.271854	-0.476434