\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Gaussian 16: AS64L-G16RevA.03 25-Dec-2016

9-Oct-2018

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

-----------------------------------

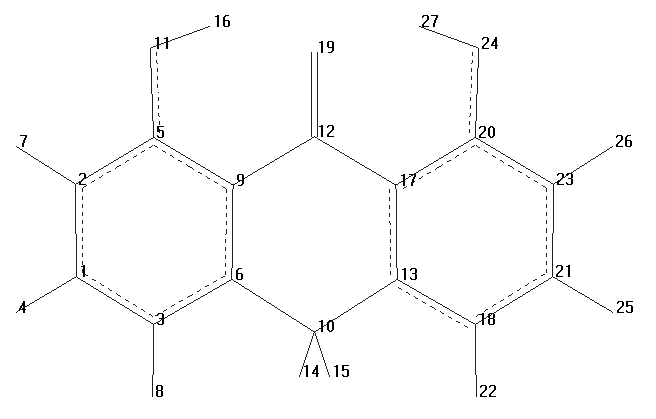
#t td(nst=60) cam-b3lyp/aug-cc-pvtz

-----------------------------------

------------------------------------------

Anthralin (B3LYP/6-31+G(d,p) C2v geometry)

------------------------------------------



Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.000000 3.707461 -1.207892

2 6 0 0.000000 3.715894 0.181479

3 6 0 0.000000 2.503691 -1.923696

4 1 0 0.000000 4.650907 -1.746528

5 6 0 0.000000 2.503501 0.883485

6 6 0 0.000000 1.286120 -1.247331

7 1 0 0.000000 4.640645 0.748108

8 1 0 0.000000 2.517286 -3.010018

9 6 0 0.000000 1.267524 0.168001

10 6 0 0.000000 -0.000000 -2.036891

11 8 0 0.000000 2.555864 2.225167

12 6 0 0.000000 0.000000 0.895659

13 6 0 -0.000000 -1.286120 -1.247331

14 1 0 -0.872070 0.000000 -2.705091

15 1 0 0.872070 -0.000000 -2.705091

16 1 0 0.000000 1.621621 2.554180

17 6 0 -0.000000 -1.267524 0.168001

18 6 0 -0.000000 -2.503691 -1.923696

19 8 0 0.000000 0.000000 2.164359

20 6 0 -0.000000 -2.503501 0.883485

21 6 0 -0.000000 -3.707461 -1.207892

22 1 0 -0.000000 -2.517286 -3.010018

23 6 0 -0.000000 -3.715894 0.181479

24 8 0 -0.000000 -2.555864 2.225167

25 1 0 -0.000000 -4.650907 -1.746528

26 1 0 -0.000000 -4.640645 0.748108

27 1 0 -0.000000 -1.621621 2.554180

---------------------------------------------------------------------

1012 basis functions, 1494 primitive gaussians, 1185 cartesian basis functions

59 alpha electrons 59 beta electrons

SCF Done: E(RCAM-B3LYP) = -765.129535612 A.U. after 12 cycles

NFock= 12 Conv=0.85D-08 -V/T= 2.0061

Excitation energies and oscillator strengths:

--------------------------------------------------

MO parentages added, p = pi, s = sigma. /JS-L

3500 cm-1 subtracted from the computed wavenumbers

--------------------------------------------------

Excited State 1: 1 Singlet-B2 27.65557 1000/cm f=0.2876

58 -> 60 0.68434 94% [4a2(p)-->7b1(p\*)]

59 -> 62 -0.10775

Excited State 2: 2 Singlet-A1 27.94835 1000/cm f=0.0267

58 -> 62 -0.13426

59 -> 60 0.68263 93% [6b1(p)-->7b1(p\*)]

Excited State 3: 1 Singlet-A2 30.88098 1000/cm f=0.0000

55 -> 60 0.68295 93% [22b2(s)-->7b1(p\*)]

55 -> 78 -0.11160

Excited State 4: 2 Singlet-B2 34.64194 1000/cm f=0.0836

57 -> 60 0.62757 79% [3a2(p)-->7b1(p\*)]

58 -> 63 0.11486

59 -> 62 0.25187 13% [6b1(p)-->5a2(p\*)]

Excited State 5: 3 Singlet-A1 38.64809 1000/cm f=0.0302

56 -> 60 0.60277 73% [5b1(p)-->7b1(p\*)]

58 -> 69 -0.18377

59 -> 63 0.25900 13% [6b1(p)-->8b1(p\*)]

Excited State 6: 3 Singlet-B2 40.9379 1000/cm f=0.1775

57 -> 60 -0.29475 17% [3a2(p)-->7b1(p\*)]

57 -> 63 0.13348

58 -> 60 0.13862

58 -> 63 0.24797 12% [4a2(p)-->8b1(p\*)]

59 -> 62 0.52064 54% [6b1(p)-->5a2(p\*)]

Excited State 7: 4 Singlet-A1 41.10647 1000/cm f=0.0013

56 -> 63 0.14443

57 -> 69 -0.16044

58 -> 62 0.60379 73% [4a2(p)-->5a2(p\*)]

59 -> 60 0.15884

59 -> 63 -0.15406

59 -> 78 -0.13014

Excited State 8: 5 Singlet-A1 43.17447 1000/cm f=0.2305

56 -> 60 -0.32677 21% [5b1(p)-->7b1(p\*)]

57 -> 62 -0.16875

58 -> 62 0.11811

58 -> 69 -0.19605

59 -> 63 0.52959 56% [6b1(p)-->8b1(p\*)]

59 -> 68 -0.10226

Excited State 9: 1 Singlet-B1 43.19061 1000/cm f=0.0009

58 -> 64 0.23628 11% [4a2(p)-->23b2(s\*)]

59 -> 61 0.59829 72% [6b1(p)-->28a1(s\*)]

59 -> 66 -0.14602

59 -> 70 -0.10345

Excited State 10: 4 Singlet-B2 43.485 1000/cm f=0.0265

56 -> 62 -0.11502

57 -> 63 -0.12580

58 -> 63 0.52311 55% [4a2(p)-->8b1(p\*)]

59 -> 62 -0.21308

59 -> 69 -0.34225 23% [6b1(p)-->6a2(p\*)]

Excited State 11: 2 Singlet-A2 43.77939 1000/cm f=0.0000

58 -> 61 0.54640 60% [4a2(p)-->28a1(s\*)]

58 -> 65 0.12229

58 -> 66 -0.16320

59 -> 64 0.30920 19% [6b1(p)-->23b2(s\*)]

59 -> 72 0.10008

Excited State 12: 5 Singlet-B2 47.41291 1000/cm f=0.5209

56 -> 62 0.20879

56 -> 69 -0.15501

57 -> 63 0.38094 29% [3a2(p)-->8b1(p\*)]

57 -> 68 -0.14284

58 -> 63 0.26079 14% [4a2(p)-->8b1(p\*)]

59 -> 62 -0.27685 15% [6b1(p)-->5a2(p\*)]

59 -> 69 0.30900 19% [6b1(p)-->6a2(p\*)]

Excited State 13: 3 Singlet-A2 47.55406 1000/cm f=0.0000

57 -> 61 -0.12273

58 -> 66 0.47217 45% [4a2(p)-->30a1(s\*)]

58 -> 71 0.11068

59 -> 64 0.41047 34% [6b1(p)-->23b2(s\*)]

59 -> 82 -0.11240

Excited State 14: 2 Singlet-B1 47.88556 1000/cm f=0.0011

58 -> 64 0.28913 17% [4a2(p)-->23b2(s\*)]

58 -> 67 0.13032

58 -> 74 -0.11488

58 -> 82 -0.10231

59 -> 65 -0.12120

59 -> 66 0.52544 55% [6b1(p)-->30a1(s\*)]

59 -> 70 0.12955

59 -> 71 0.11447

Excited State 15: 3 Singlet-B1 48.15333 1000/cm f=0.0027

58 -> 64 0.30865 19% [4a2(p)-->23b2(s\*)]

58 -> 67 -0.21429

59 -> 61 -0.18787

59 -> 65 0.51147 52% [6b1(p)-->29a1(s\*)]

59 -> 77 -0.10447

Excited State 16: 4 Singlet-A2 48.65259 1000/cm f=0.0000

58 -> 61 -0.28742 17% [4a2(p)-->28a1(s\*)]

58 -> 65 0.45065 41% [4a2(p)-->29a1(s\*)]

58 -> 66 -0.11620

59 -> 64 0.19942

59 -> 67 -0.29517 17% [6b1(p)-->24b2(s\*)]

Excited State 17: 6 Singlet-A1 49.16555 1000/cm f=0.0026

56 -> 63 -0.10753

57 -> 62 0.38216 29% [3a2(p)-->5a2(p\*)]

58 -> 62 0.10790

58 -> 69 0.30093 18% [4a2(p)-->6a2(p\*)]

58 -> 75 0.10847

59 -> 63 0.30275 18% [6b1(p)-->8b1(p\*)]

59 -> 68 0.31320 20% [6b1(p)-->9b1(p\*)]

Excited State 18: 4 Singlet-B1 50.01244 1000/cm f=0.0008

51 -> 62 0.10983

53 -> 60 -0.46206 43% [27a1(s)-->7b1(p\*)]

55 -> 62 0.48809 48% [22b2(s)-->5a2(p\*)]

55 -> 69 0.11939

Excited State 19: 7 Singlet-A1 50.8932 1000/cm f=0.0579

54 -> 60 -0.10195

56 -> 63 0.28284 16% [5b1(p)-->8b1(p\*)]

57 -> 69 -0.20223

58 -> 62 -0.14143

58 -> 69 -0.22816 10% [4a2(p)-->6a2(p\*)]

58 -> 75 0.16202

59 -> 68 0.46428 43% [6b1(p)-->9b1(p\*)]

Excited State 20: 6 Singlet-B2 51.02386 1000/cm f=0.0141

57 -> 63 -0.13451

58 -> 63 0.14870

58 -> 68 0.58464 68% [4a2(p)-->9b1(p\*)]

58 -> 73 0.13233

59 -> 75 0.22798 10% [6b1(p)-->7a2(p\*)]

Excited State 21: 5 Singlet-A2 51.51585 1000/cm f=0.0000

56 -> 64 0.15323

57 -> 61 0.47219 45% [3a2(p)-->28a1(s\*)]

57 -> 66 -0.13915

57 -> 70 -0.11546

58 -> 61 0.12944

58 -> 65 0.23568 11% [4a2(p)-->29a1(s\*)]

58 -> 66 0.19807

59 -> 67 -0.13676

59 -> 72 -0.15599

59 -> 74 -0.10353

Excited State 22: 5 Singlet-B1 51.62393 1000/cm f=0.0141

50 -> 60 0.10893

53 -> 60 0.31828 20% [27a1(s)-->7b1(p\*)]

55 -> 62 0.29978 18% [22b2(s)-->5a2(p\*)]

56 -> 61 -0.21549

57 -> 64 -0.20634

58 -> 64 -0.25412 13% [4a2(p)-->23b2(s\*)]

58 -> 67 -0.12805

58 -> 72 -0.10841

59 -> 61 0.12561

59 -> 65 0.14242

59 -> 66 0.11729

Excited State 23: 6 Singlet-B1 51.66507 1000/cm f=0.0130

50 -> 60 0.12019

53 -> 60 0.35460 25% [27a1(s)-->7b1(p\*)]

55 -> 62 0.34179 23% [22b2(s)-->5a2(p\*)]

56 -> 61 0.18673

57 -> 64 0.18250

58 -> 64 0.23022 11% [4a2(p)-->23b2(s\*)]

58 -> 67 0.12345

59 -> 61 -0.11434

59 -> 65 -0.11777

59 -> 66 -0.10785

Excited State 24: 6 Singlet-A2 51.70217 1000/cm f=0.0000

51 -> 60 0.64972 84% [21b2(s)-->7b1(p\*)]

53 -> 62 -0.14902

Excited State 25: 8 Singlet-A1 52.099 1000/cm f=0.1741

54 -> 60 -0.30876 19% [4b1(p)-->7b1(p\*)]

56 -> 63 0.32370 21% [5b1(p)-->8b1(p\*)]

57 -> 62 0.27833 15% [3a2(p)-->5a2(p\*)]

57 -> 69 -0.19496

58 -> 62 -0.17037

59 -> 63 0.10122

59 -> 68 -0.29447 17% [6b1(p)-->9b1(p\*)]

Excited State 26: 7 Singlet-B2 52.3337 1000/cm f=0.0048

56 -> 62 0.50377 51% [5b1(p)-->5a2(p\*)]

57 -> 63 0.11548

58 -> 63 -0.14085

59 -> 69 -0.43390 38% [6b1(p)-->6a2(p\*)]

Excited State 27: 8 Singlet-B2 52.54663 1000/cm f=0.1608

56 -> 62 -0.38070 29% [5b1(p)-->5a2(p\*)]

56 -> 69 -0.11932

57 -> 63 0.41332 34% [3a2(p)-->8b1(p\*)]

57 -> 68 -0.10659

58 -> 63 -0.14313

58 -> 68 0.18348

59 -> 69 -0.26227 14% [6b1(p)-->6a2(p\*)]

59 -> 75 0.10210

Excited State 28: 7 Singlet-A2 52.6531 1000/cm f=0.0000

55 -> 63 0.62019 77% [22b2(s)-->8b1(p\*)]

55 -> 68 -0.21693

Excited State 29: 8 Singlet-A2 52.67729 1000/cm f=0.0000

57 -> 61 0.20828

57 -> 65 0.10213

57 -> 66 -0.14015

58 -> 61 -0.21573

58 -> 66 -0.15609

58 -> 71 -0.26177 14% [4a2(p)-->32a1(s\*)]

59 -> 64 0.25502 13% [6b1(p)-->23b2(s\*)]

59 -> 67 0.40714 33% [6b1(p)-->24b2(s\*)]

Excited State 30: 9 Singlet-A1 52.77247 1000/cm f=0.4129

56 -> 63 0.18493

57 -> 62 -0.38995 30% [3a2(p)-->5a2(p\*)]

58 -> 69 0.51391 53% [4a2(p)-->6a2(p\*)]

59 -> 63 0.10226

Excited State 31: 7 Singlet-B1 53.03379 1000/cm f=0.0001

58 -> 67 -0.22921 11% [4a2(p)-->24b2(s\*)]

58 -> 72 0.16685

58 -> 76 -0.12746

59 -> 70 0.50001 50% [6b1(p)-->31a1(s\*)]

59 -> 71 0.22908 10% [6b1(p)-->32a1(s\*)]

Excited State 32: 9 Singlet-A2 53.48627 1000/cm f=0.0000

58 -> 66 -0.10335

58 -> 70 0.59344 70% [4a2(p)-->31a1(s\*)]

58 -> 86 -0.10662

59 -> 72 0.16219

59 -> 76 -0.16747

Excited State 33: 8 Singlet-B1 54.07989 1000/cm f=0.0009

57 -> 64 -0.13401

58 -> 67 0.39560 31% [4a2(p)-->24b2(s\*)]

58 -> 76 -0.10463

59 -> 65 0.18509

59 -> 70 0.33617 23% [6b1(p)-->31a1(s\*)]

59 -> 71 -0.31899 20% [6b1(p)-->32a1(s\*)]

Excited State 34: 10 Singlet-A2 54.45171 1000/cm f=0.0000

57 -> 61 -0.23122 11% [3a2(p)-->28a1(s\*)]

57 -> 65 0.13446

57 -> 66 0.16329

58 -> 61 0.12390

58 -> 65 0.36463 27% [4a2(p)-->29a1(s\*)]

58 -> 66 0.18290

58 -> 71 -0.20007

59 -> 64 -0.23359 11% [6b1(p)-->23b2(s\*)]

59 -> 67 0.24521 12% [6b1(p)-->24b2(s\*)]

59 -> 72 -0.13400

Excited State 35: 9 Singlet-B1 54.71384 1000/cm f=0.0008

56 -> 61 0.40167 32% [5b1(p)-->28a1(s\*)]

56 -> 66 -0.24373 12% [5b1(p)-->30a1(s\*)]

56 -> 70 -0.10813

57 -> 64 0.12308

58 -> 64 -0.28049 16% [4a2(p)-->23b2(s\*)]

58 -> 72 -0.12269

59 -> 61 0.16517

59 -> 65 0.17823

59 -> 66 0.19071

Excited State 36: 11 Singlet-A2 55.21955 1000/cm f=0.0000

56 -> 64 0.22138 10% [5b1(p)-->23b2(s\*)]

57 -> 61 0.20463

57 -> 66 0.32784 21% [3a2(p)-->30a1(s\*)]

58 -> 66 0.15099

59 -> 72 0.34667 24% [6b1(p)-->25b2(s\*)]

59 -> 74 0.24030 12% [6b1(p)-->26b2(s\*)]

Excited State 37: 10 Singlet-A1 55.3236 1000/cm f=0.0857

54 -> 60 0.57342 66% [4b1(p)-->7b1(p\*)]

56 -> 63 0.24378 12% [5b1(p)-->8b1(p\*)]

57 -> 62 0.24354 12% [3a2(p)-->5a2(p\*)]

Excited State 38: 10 Singlet-B1 56.06401 1000/cm f=0.0056

56 -> 66 0.25926 13% [5b1(p)-->30a1(s\*)]

57 -> 64 0.33667 23% [3a2(p)-->23b2(s\*)]

58 -> 72 -0.30705 19% [4a2(p)-->25b2(s\*)]

58 -> 74 -0.26868 14% [4a2(p)-->26b2(s\*)]

59 -> 65 0.17106

59 -> 66 -0.15133

Excited State 39: 9 Singlet-B2 56.26727 1000/cm f=0.1434

52 -> 60 0.50158 50% [2a2(p)-->7b1(p\*)]

54 -> 62 0.12654

55 -> 61 0.20236

55 -> 65 0.12247

55 -> 66 -0.24450 12% [22b2(s)-->30a1(s\*)]

57 -> 68 0.14332

59 -> 75 -0.16073

Excited State 40: 11 Singlet-B1 56.47052 1000/cm f=0.0011

50 -> 60 0.22898 10% [26a1(s)-->7b1(p\*)]

50 -> 63 0.11024

53 -> 60 0.10877

53 -> 63 -0.14127

55 -> 69 0.59201 70% [22b2(s)-->6a2(p\*)]

Excited State 41: 10 Singlet-B2 56.48262 1000/cm f=0.0024

52 -> 60 0.26976 15% [2a2(p)-->7b1(p\*)]

55 -> 61 -0.33240 22% [22b2(s)-->28a1(s\*)]

55 -> 65 -0.19962

55 -> 66 0.37715 28% [22b2(s)-->30a1(s\*)]

55 -> 71 0.13487

55 -> 79 -0.10776

57 -> 68 0.11415

59 -> 75 -0.14994

Excited State 42: 12 Singlet-B1 56.92783 1000/cm f=0.0017

56 -> 61 0.18031

56 -> 65 -0.15018

56 -> 66 -0.14777

57 -> 64 -0.20605

57 -> 67 0.16326

58 -> 67 0.29060 17% [4a2(p)-->24b2(s\*)]

58 -> 72 0.10086

58 -> 74 -0.18900

59 -> 66 -0.16279

59 -> 71 0.34367 24% [6b1(p)-->32a1(s\*)]

Excited State 43: 11 Singlet-B2 57.00849 1000/cm f=0.0044

52 -> 60 0.30431 19% [2a2(p)-->7b1(p\*)]

56 -> 69 -0.14869

57 -> 63 -0.19939

57 -> 68 -0.28052 16% [3a2(p)-->9b1(p\*)]

58 -> 68 -0.15876

58 -> 80 -0.16470

59 -> 75 0.40444 33% [6b1(p)-->7a2(p\*)]

Excited State 44: 12 Singlet-A2 57.05527 1000/cm f=0.0000

56 -> 67 -0.10887

57 -> 65 0.29016 17% [3a2(p)-->29a1(s\*)]

58 -> 65 0.15374

58 -> 70 -0.15600

58 -> 71 0.39463 31% [4a2(p)-->32a1(s\*)]

59 -> 67 0.12297

59 -> 72 0.23278 11% [6b1(p)-->25b2(s\*)]

59 -> 74 -0.22191 10% [6b1(p)-->26b2(s\*)]

Excited State 45: 11 Singlet-A1 57.55694 1000/cm f=0.0050

56 -> 68 0.12747

58 -> 75 0.38830 30% [4a2(p)-->7a2(p\*)]

58 -> 84 0.15432

59 -> 68 -0.20404

59 -> 73 0.45693 42% [6b1(p)-->10b1(p\*)]

59 -> 80 -0.13754

Excited State 46: 13 Singlet-B1 57.74406 1000/cm f=0.0009

56 -> 65 -0.12052

56 -> 66 0.25904 13% [5b1(p)-->30a1(s\*)]

57 -> 64 0.23386 11% [3a2(p)-->23b2(s\*)]

57 -> 67 0.12050

58 -> 64 -0.19590

58 -> 67 0.12020

58 -> 72 0.36138 26% [4a2(p)-->25b2(s\*)]

58 -> 74 0.12475

59 -> 65 0.12231

59 -> 66 0.17832

59 -> 71 0.11461

59 -> 77 -0.14643

59 -> 87 0.10012

Excited State 47: 12 Singlet-A1 57.88037 1000/cm f=0.0811

54 -> 63 -0.10672

56 -> 63 0.38090 29% [5b1(p)-->8b1(p\*)]

57 -> 69 0.51909 54% [3a2(p)-->6a2(p\*)]

59 -> 73 -0.10238

59 -> 78 0.11479

Excited State 48: 12 Singlet-B2 57.99571 1000/cm f=0.0095

58 -> 68 -0.10516

58 -> 73 0.59371 70% [4a2(p)-->10b1(p\*)]

58 -> 78 -0.17146

58 -> 80 0.15659

59 -> 84 0.13863

Excited State 49: 13 Singlet-A2 58.27478 1000/cm f=0.0000

56 -> 64 0.21101

57 -> 66 0.35795 26% [3a2(p)-->30a1(s\*)]

57 -> 70 0.12490

58 -> 66 -0.23574 11% [4a2(p)-->30a1(s\*)]

58 -> 77 0.14463

59 -> 64 0.18623

59 -> 72 -0.30073 18% [6b1(p)-->25b2(s\*)]

59 -> 74 -0.19259

Excited State 50: 14 Singlet-A2 58.47157 1000/cm f=0.0000

56 -> 64 0.17488

56 -> 67 -0.11286

57 -> 61 -0.15476

57 -> 65 0.44797 40% [3a2(p)-->29a1(s\*)]

57 -> 66 -0.10299

57 -> 77 -0.11179

58 -> 65 -0.17275

58 -> 71 -0.15635

59 -> 64 0.10582

59 -> 67 -0.26364 14% [6b1(p)-->24b2(s\*)]

59 -> 74 0.12813

Excited State 51: 13 Singlet-A1 58.7329 1000/cm f=0.0191

57 -> 69 0.13810

58 -> 75 -0.37744 28% [4a2(p)-->7a2(p\*)]

59 -> 73 0.42615 36% [6b1(p)-->10b1(p\*)]

59 -> 80 0.34109 23% [6b1(p)-->12b1(p\*)]

Excited State 52: 15 Singlet-A2 58.8926 1000/cm f=0.0000

49 -> 60 0.61669 76% [20b2(s)-->7b1(p\*)]

50 -> 62 0.20460

53 -> 62 0.16536

55 -> 63 0.11059

Excited State 53: 13 Singlet-B2 58.91599 1000/cm f=0.0461

56 -> 69 0.50383 51% [5b1(p)-->6a2(p\*)]

57 -> 63 0.21252

57 -> 68 0.16027

58 -> 68 -0.16048

58 -> 73 0.11148

58 -> 80 -0.18906

59 -> 75 0.22906 10% [6b1(p)-->7a2(p\*)]

Excited State 54: 14 Singlet-B1 59.58866 1000/cm f=0.0026

56 -> 61 -0.30887 19% [5b1(p)-->28a1(s\*)]

56 -> 65 0.36009 26% [5b1(p)-->29a1(s\*)]

56 -> 66 -0.17476

56 -> 77 -0.10522

57 -> 64 0.16493

57 -> 67 -0.19837

57 -> 74 0.11590

58 -> 67 0.16732

58 -> 72 0.13065

59 -> 65 0.16933

59 -> 71 0.15525

59 -> 77 0.10092

Excited State 55: 14 Singlet-B2 59.60559 1000/cm f=0.0028

56 -> 69 -0.20978

58 -> 73 0.13877

58 -> 78 0.54364 59% [4a2(p)-->11b1(p\*)]

58 -> 80 -0.20223

59 -> 75 -0.11295

59 -> 84 0.14630

Excited State 56: 16 Singlet-A2 59.93467 1000/cm f=0.0000

57 -> 66 -0.11506

57 -> 70 0.12684

57 -> 71 0.11125

58 -> 70 0.16048

58 -> 71 0.26646 14% [4a2(p)-->32a1(s\*)]

58 -> 77 0.12699

58 -> 81 0.13532

59 -> 67 0.12622

59 -> 72 -0.22625 10% [6b1(p)-->25b2(s\*)]

59 -> 74 0.30939 19% [6b1(p)-->26b2(s\*)]

59 -> 76 0.28410 16% [6b1(p)-->27b2(s\*)]

Excited State 57: 14 Singlet-A1 59.99032 1000/cm f=0.0598

57 -> 69 -0.15018

58 -> 75 -0.12605

58 -> 84 0.12819

59 -> 78 0.58958 70% [6b1(p)-->11b1(p\*)]

59 -> 80 -0.20155

Excited State 58: 15 Singlet-B2 60.08388 1000/cm f=0.0033

56 -> 69 -0.29323 17% [5b1(p)-->6a2(p\*)]

56 -> 75 0.10714

57 -> 68 0.50600 51% [3a2(p)-->9b1(p\*)]

58 -> 73 -0.11975

58 -> 78 -0.13106

58 -> 80 -0.15930

59 -> 75 0.22154 10% [6b1(p)-->7a2(p\*)]

Excited State 59: 15 Singlet-B1 60.18712 1000/cm f=0.0126

58 -> 67 0.12806

58 -> 72 -0.29556 17% [4a2(p)-->25b2(s\*)]

58 -> 74 0.29802 18% [4a2(p)-->26b2(s\*)]

58 -> 76 0.33379 22% [4a2(p)-->27b2(s\*)]

58 -> 82 0.11997

59 -> 70 0.16850

59 -> 71 0.16064

59 -> 81 0.19593

Excited State 60: 16 Singlet-B1 60.24358 1000/cm f=0.0006

47 -> 60 -0.11630

49 -> 62 0.16087

50 -> 60 0.55859 62% [26a1(s)-->7b1(p\*)]

51 -> 62 0.16857

55 -> 62 -0.17333

55 -> 69 -0.20904

Orbital symmetries:

---------------------

Numbering added /JS-L

---------------------

Occupied (1B2) (1A1) (2A1) (3A1) (2B2) (4A1) (3B2) (5A1) (6A1) (4B2)

(7A1) (8A1) (5B2) (6B2) (9A1) (10A1) (7B2) (11A1) (8B2) (12A1)

(13A1) (9B2) (14A1) (15A1) (10B2) (11B2) (16A1) (17A1) (12B2) (18A1)

(13B2) (19A1) (14B2) (15B2) (20A1) (21A1) (22A1) (16B2) (1B1) (17B2)

(23A1) (2B1) (18B2) (1A2) (24A1) (19B2) (25A1) (3B1) (20B2) (26A1)

(21B2) (2A2) (27A1) (4B1) (22B2) (5B1) (3A2) (4A2) (6B1)

Virtual (7B1) (28A1) (5A2) (8B1) (23B2) (29A1) (30A1) (24B2) (9B1) (6A2)

(31A1) (32A1) (25B2) (10B1) (26B2) (7A2) (27B2) (33A1) (11B1) (34A1)

(12B1) (35A1) (28B2) (36A1) (8A2) (29B2) (37A1) (38A1) (39A1) (30B2)

(B1) (B2) (A1) (A2) (B1) (B2) (B1) (A1) (B2) (A2)

(A1) (B2) (A2) (B2) (B1) (B1) (A1) (A1) (A1) (B2)

(B1) (A1) (A1) (B2) (A2) (A1) (B1) (B2) (A1) (B1)

(A2) (B2) (A1) (B2) (B2) (A2) (A1) (B2) (A1) (B1)

(A2) (A1) (A1) (B2) (A1) (B2) (B2) (A1) (A1) (B2)

(B1) (B2) (A1) (A2) (B2) (A1) (B1) (A1) (B2) (B1)

(A1) (A1) (B2) (A2) (B1) (A1) (B2) (A1) (A2) (B2)

(A1) (A1) (B1) (B1) (B2) (A2) (A2) (A2) (A1) (B1)

(B2) (B1) (A2) (B2) (A1) (A1) (B2) (B1) (B1) (A1)

(B2) (B2) (A1) (B2) (A1) (A1) (A2) (B2) (B1) (B2)

(A1) (A1) (A2) (B2) (A1) (A1) (B1) (A1) (B2) (B1)

(A1) (B2) (B2) (A1) (B1) (B2) (A2) (B2) (B1) (A1)

(B2) (A1) (B1) (A1) (B2) (A2) (A1) (A2) (B2) (A1)

(B2) (A1) (B2) (A2) (B1) (B2) (A1) (A1) (A2) (B1)

(B2) (A1) (B2) (B1) (A1) (B2) (A1) (A2) (A1) (B2)

(A1) (B2) (B1) (A1) (B1) (A2) (A1) (B2) (A1) (B2)

(A1) (A2) (B2) (B2) (A1) (B1) (A1) (A2) (B2) (B2)

(B2) (A2) (B1) (A1) (A1) (A1) (B1) (A2) (B2) (A2)

(B1) (A1) (B2) (A1) (B1) (A2) (B2) (A1) (B1) (A1)

(A2) (B1) (B2) (A1) (B2) (B1) (A1) (B2) (A2) (A1)

(B2) (A1) (B1) (A2) (A1) (B1) (B2) (B2) (B1) (A1)

(A2) (B1) (A1) (A2) (B2) (A1) (B1) (B2) (A2) (A1)

(B2) (A1) (B1) (B1) (B2) (A1) (B1) (B2) (A2) (A1)

(B1) (A2) (A2) (A1) (B2) (B2) (A1) (A2) (B1) (A1)

(B2) (A2) (B1) (B2) (A2) (B2) (A1) (B1) (B2) (A1)

(A1) (B2) (B2) (B1) (A1) (A2) (B1) (A1) (A1) (B2)

(A2) (A1) (B2) (A2) (B2) (A1) (B2) (B1) (A1) (A2)

(B2) (B1) (A1) (B1) (A1) (A2) (B2) (B2) (A1) (B1)

(A1) (B1) (B2) (A2) (B2) (A1) (B2) (A2) (A1) (A1)

(B1) (B2) (A1) (B2) (B1) (A1) (A1) (A2) (B2) (A1)

(B2) (A2) (A1) (B1) (A2) (A1) (B2) (B2) (B1) (A2)

(B2) (A1) (B1) (A1) (A1) (A2) (B2) (B1) (A1) (A2)

(B1) (A1) (B2) (B2) (A2) (B2) (B1) (A1) (A2) (A1)

(B2) (A1) (B1) (A1) (B2) (A1) (B1) (B2) (B2) (A2)

(A1) (B1) (B2) (A2) (B2) (A1) (A1) (B2) (A2) (A1)

(B2) (B1) (A1) (A2) (B1) (B2) (B1) (A2) (B2) (B1)

(A1) (A1) (B1) (A1) (B2) (A2) (B1) (B2) (A1) (B1)

(B2) (B1) (A2) (A1) (B2) (A1) (B2) (A2) (A1) (A1)

(B1) (B2) (B2) (B2) (A2) (A1) (B1) (A2) (A1) (B2)

(A1) (B1) (A1) (B2) (A2) (B1) (A1) (B1) (A2) (A1)

(A1) (B2) (B2) (A1) (B2) (B1) (A2) (A1) (A2) (B2)

(B1) (A1) (B2) (B1) (A2) (A1) (B2) (A1) (A2) (B2)

(B2) (A1) (B1) (A1) (B2) (A2) (A1) (B1) (B2) (A1)

(A2) (B2) (A1) (B1) (B2) (B2) (A2) (A1) (B1) (A1)

(B2) (B2) (B1) (A1) (A1) (B2) (A2) (B2) (B1) (A1)

(B2) (A1) (B2) (B1) (A1) (A2) (B2) (A2) (B1) (A1)

(A2) (B2) (A1) (A2) (A1) (B1) (A1) (B2) (B2) (A2)

(B1) (A1) (A1) (B2) (B2) (A2) (B1) (A1) (A2) (B2)

(A1) (B1) (B2) (A2) (A1) (B2) (B1) (A1) (B2) (B1)

(A1) (A1) (A2) (B2) (B1) (B2) (A1) (A1) (B2) (B1)

(A2) (B2) (A2) (B2) (B1) (A1) (A1) (A1) (B2) (A1)

(B1) (B2) (A2) (A1) (B2) (A2) (B2) (A1) (B1) (B2)

(A1) (A2) (B1) (A1) (B2) (A2) (B2) (B1) (A1) (A1)

(A2) (A1) (B2) (B2) (B1) (A1) (A2) (B1) (A1) (B1)

(A1) (A2) (B2) (B2) (B1) (B2) (A2) (B1) (A2) (A1)

(A1) (A2) (B2) (A1) (B1) (A2) (B1) (B2) (A1) (B1)

(B2) (A1) (A2) (A2) (B2) (A1) (B1) (B2) (B1) (A1)

(A1) (B1) (B2) (A1) (B1) (A2) (B1) (A1) (A2) (B2)

(A1) (B2) (B1) (A2) (B1) (A1) (B2) (A2) (B1) (A2)

(A1) (B2) (B2) (A1) (A2) (B2) (A2) (B1) (A1) (B2)

(A1) (B1) (B2) (A1) (A1) (B2) (B1) (A2) (B2) (B1)

(A1) (B2) (A1) (A2) (A1) (B2) (A2) (B1) (B2) (B1)

(A2) (A1) (A1) (B2) (B1) (A1) (B2) (B2) (A1) (A2)

(A1) (B2) (B1) (B1) (B1) (B2) (A1) (A2) (A1) (B2)

(A1) (A2) (B1) (A1) (B2) (A1) (B1) (B2) (A1) (A2)

(B2) (B2) (A1) (B2) (A2) (B2) (B1) (A1) (A1) (B2)

(A1) (A2) (B1) (B1) (B2) (A2) (A1) (A1) (B2) (B1)

(B2) (A1) (A2) (A1) (B1) (B2) (A2) (A1) (A2) (B2)

(B1) (A1) (B2) (A2) (A1) (B1) (B2) (A1) (A2) (B1)

(B2) (B1) (B2) (A1) (A2) (B1) (A1) (B2) (A2) (B1)

(A2) (A1) (B2) (B2) (A1) (B2) (A1) (B1) (A2) (B2)

(B1) (A2) (A1) (B2) (A1) (B1) (A1) (B2) (A2) (B2)

(A1) (B1) (A1) (A2) (A1) (B2) (B1) (B1) (A2) (B2)

(A1) (B1) (A2) (B2) (A1) (A2) (A1) (A1) (B1) (B2)

(B2) (A2) (B1) (B2) (A1) (B1) (A1) (A2) (A1) (B2)

(B2) (B1) (A1) (B2) (A2) (A1) (A1) (B1) (A1) (B2)

(B1) (A2) (B2) (A2) (B1) (A1) (B2) (A2) (A1) (B2)

(A1) (B1) (B2) (A1) (B1) (A2) (B2) (A1) (B2) (A2)

(A1) (B1) (B2) (A2) (A1) (B1) (B2) (A2) (B2) (B1)

(A1) (A1) (B2) (A2) (B2) (B1) (A1) (B1) (A2) (B2)

(B1) (A1) (B2) (A1) (B2) (A1) (B2) (A1) (B2) (A2)

(B1) (A1) (B2) (A1) (A2) (B2) (A1) (B2) (A1) (B2)

(B2) (A1) (A1) (A1) (B2) (A1) (B1) (B2) (B2) (A1)

(A1) (B2) (A1) (A1) (B2) (A1) (B2) (B2) (A1) (B2)

(A1) (B2) (A1) (B2) (A1) (B2) (A1) (B2) (A1) (A1)

(B2) (B2) (B1) (A1) (A2) (B1) (B1) (B2) (A1) (A2)

(B2) (A1) (B1) (A2) (B1) (A1) (B2) (A2) (A1) (B1)

(B2) (A2) (A1) (A2) (B1) (B2) (A1) (B2) (A1) (B1)

(A2) (B1) (A1) (B2) (B2) (A1) (A1) (B2) (A1) (B2)

(A1) (B2) (A1) (B2) (A1) (B2) (A1) (B2) (A1) (B2)

(A1) (A1) (B2) (A1) (B2) (A1) (B2) (A1) (A1) (B2)

(A1)

The electronic state is 1-A1.

Alpha occ. eigenvalues -- -19.22813 -19.22813 -19.21689 -10.36871 -10.33796

Alpha occ. eigenvalues -- -10.33796 -10.29265 -10.29264 -10.28129 -10.27743

Alpha occ. eigenvalues -- -10.27743 -10.27709 -10.27709 -10.26015 -10.26014

Alpha occ. eigenvalues -- -10.25837 -10.25837 -1.16489 -1.14925 -1.12371

Alpha occ. eigenvalues -- -0.97669 -0.95100 -0.89682 -0.86555 -0.84748

Alpha occ. eigenvalues -- -0.83598 -0.79299 -0.74143 -0.73203 -0.68810

Alpha occ. eigenvalues -- -0.68314 -0.65603 -0.61661 -0.61165 -0.60735

Alpha occ. eigenvalues -- -0.56651 -0.55623 -0.55285 -0.54699 -0.52814

Alpha occ. eigenvalues -- -0.51829 -0.50995 -0.49943 -0.49638 -0.49443

Alpha occ. eigenvalues -- -0.47661 -0.47046 -0.46173 -0.45245 -0.44838

Alpha occ. eigenvalues -- -0.42299 -0.42142 -0.41905 -0.40877 -0.34710

Alpha occ. eigenvalues -- -0.33787 -0.32703 -0.29123 -0.28887

Alpha virt. eigenvalues -- -0.05088 0.00267 0.00799 0.01028 0.01114

Alpha virt. eigenvalues -- 0.01904 0.02321 0.02880 0.03115 0.03564

Alpha virt. eigenvalues -- 0.03990 0.04333 0.04486 0.06314 0.06314

Alpha virt. eigenvalues -- 0.06358 0.06784 0.06927 0.08016 0.08193

Alpha virt. eigenvalues -- 0.08344 0.08367 0.08525 0.09011 0.09303

Alpha virt. eigenvalues -- 0.09676 0.10127 0.10500 0.10820 0.11069

Alpha virt. eigenvalues -- 0.11233 0.11282 0.11390 0.11477 0.11907

Alpha virt. eigenvalues -- 0.12343 0.12371 0.12775 0.13473 0.13771

Alpha virt. eigenvalues -- 0.14874 0.14884 0.15404 0.15552 0.15858

Alpha virt. eigenvalues -- 0.16211 0.16403 0.16456 0.17141 0.17323

Alpha virt. eigenvalues -- 0.18741 0.19036 0.19217 0.19259 0.19511

Alpha virt. eigenvalues -- 0.19669 0.20369 0.20413 0.20517 0.20927

Alpha virt. eigenvalues -- 0.20974 0.21255 0.22114 0.22275 0.22525

Alpha virt. eigenvalues -- 0.22811 0.22903 0.23306 0.23453 0.23715

Alpha virt. eigenvalues -- 0.24155 0.24264 0.24421 0.24801 0.24879

Alpha virt. eigenvalues -- 0.25347 0.25820 0.26172 0.26293 0.26429

Alpha virt. eigenvalues -- 0.27163 0.27221 0.27335 0.27449 0.28272

Alpha virt. eigenvalues -- 0.28286 0.28705 0.29666 0.29779 0.30021

Alpha virt. eigenvalues -- 0.30380 0.31083 0.31393 0.31459 0.31799

Alpha virt. eigenvalues -- 0.32101 0.32556 0.32651 0.32778 0.33818

Alpha virt. eigenvalues -- 0.34124 0.34285 0.34614 0.35011 0.35309

Alpha virt. eigenvalues -- 0.35811 0.36202 0.37108 0.37144 0.37368

Alpha virt. eigenvalues -- 0.37389 0.37842 0.37940 0.38069 0.38173

Alpha virt. eigenvalues -- 0.38763 0.38795 0.39033 0.39650 0.39803

Alpha virt. eigenvalues -- 0.39979 0.40545 0.40821 0.41098 0.41648

Alpha virt. eigenvalues -- 0.41813 0.42191 0.42703 0.42710 0.42898

Alpha virt. eigenvalues -- 0.42926 0.43597 0.43703 0.44173 0.44184

Alpha virt. eigenvalues -- 0.44634 0.45117 0.45148 0.45151 0.45297

Alpha virt. eigenvalues -- 0.45749 0.45858 0.46073 0.46193 0.46687

Alpha virt. eigenvalues -- 0.47269 0.48007 0.48098 0.48315 0.48633

Alpha virt. eigenvalues -- 0.48701 0.48800 0.49713 0.50067 0.50611

Alpha virt. eigenvalues -- 0.50655 0.50706 0.51232 0.51817 0.52451

Alpha virt. eigenvalues -- 0.52763 0.53370 0.55041 0.55146 0.55168

Alpha virt. eigenvalues -- 0.56012 0.56039 0.56821 0.57226 0.57282

Alpha virt. eigenvalues -- 0.57640 0.57648 0.58485 0.58855 0.59623

Alpha virt. eigenvalues -- 0.60964 0.61008 0.62035 0.62150 0.62210

Alpha virt. eigenvalues -- 0.62977 0.63237 0.63549 0.63877 0.66088

Alpha virt. eigenvalues -- 0.66156 0.66179 0.66225 0.66791 0.67217

Alpha virt. eigenvalues -- 0.67888 0.68236 0.68301 0.68436 0.69459

Alpha virt. eigenvalues -- 0.69679 0.70984 0.71090 0.71293 0.72157

Alpha virt. eigenvalues -- 0.72367 0.72728 0.72742 0.73671 0.74396

Alpha virt. eigenvalues -- 0.74772 0.74865 0.75066 0.75100 0.75906

Alpha virt. eigenvalues -- 0.76252 0.76669 0.76689 0.76788 0.77739

Alpha virt. eigenvalues -- 0.77743 0.77942 0.78666 0.78869 0.79180

Alpha virt. eigenvalues -- 0.79392 0.79711 0.79840 0.80762 0.81058

Alpha virt. eigenvalues -- 0.81318 0.81799 0.81867 0.82048 0.82244

Alpha virt. eigenvalues -- 0.82867 0.83295 0.83537 0.84182 0.84486

Alpha virt. eigenvalues -- 0.84909 0.85068 0.85571 0.85920 0.85970

Alpha virt. eigenvalues -- 0.85981 0.86615 0.87340 0.87434 0.87793

Alpha virt. eigenvalues -- 0.87806 0.88909 0.89184 0.89348 0.89762

Alpha virt. eigenvalues -- 0.89891 0.90422 0.91104 0.91861 0.92027

Alpha virt. eigenvalues -- 0.92298 0.93026 0.93256 0.93331 0.93808

Alpha virt. eigenvalues -- 0.94500 0.94946 0.95142 0.95774 0.96819

Alpha virt. eigenvalues -- 0.96887 0.97149 0.97546 0.97757 0.98303

Alpha virt. eigenvalues -- 0.98415 0.98828 0.98864 0.99924 1.00256

Alpha virt. eigenvalues -- 1.00461 1.00969 1.01207 1.01983 1.02227

Alpha virt. eigenvalues -- 1.02697 1.03257 1.03921 1.04060 1.04142

Alpha virt. eigenvalues -- 1.04659 1.05287 1.05804 1.06176 1.06716

Alpha virt. eigenvalues -- 1.07206 1.07606 1.07882 1.08510 1.08594

Alpha virt. eigenvalues -- 1.09202 1.09312 1.09348 1.09733 1.10447

Alpha virt. eigenvalues -- 1.10709 1.11361 1.11562 1.12247 1.12446

Alpha virt. eigenvalues -- 1.12859 1.12911 1.13764 1.14080 1.14944

Alpha virt. eigenvalues -- 1.15308 1.15635 1.15639 1.16148 1.17157

Alpha virt. eigenvalues -- 1.17396 1.18120 1.18391 1.18673 1.18903

Alpha virt. eigenvalues -- 1.19343 1.20774 1.21826 1.22571 1.22969

Alpha virt. eigenvalues -- 1.23512 1.24269 1.24713 1.25963 1.26826

Alpha virt. eigenvalues -- 1.27198 1.27292 1.27621 1.27947 1.28349

Alpha virt. eigenvalues -- 1.29707 1.30134 1.30791 1.31191 1.31389

Alpha virt. eigenvalues -- 1.31824 1.31832 1.31882 1.33283 1.33705

Alpha virt. eigenvalues -- 1.34426 1.34599 1.35289 1.35706 1.35809

Alpha virt. eigenvalues -- 1.36406 1.36599 1.37466 1.38511 1.39486

Alpha virt. eigenvalues -- 1.39524 1.39634 1.39680 1.40589 1.41071

Alpha virt. eigenvalues -- 1.41259 1.42037 1.43033 1.43619 1.44133

Alpha virt. eigenvalues -- 1.44403 1.45142 1.45239 1.46305 1.46534

Alpha virt. eigenvalues -- 1.46772 1.47798 1.48327 1.48912 1.49787

Alpha virt. eigenvalues -- 1.50043 1.50949 1.51181 1.51208 1.52688

Alpha virt. eigenvalues -- 1.52931 1.53163 1.53479 1.53874 1.54352

Alpha virt. eigenvalues -- 1.54864 1.55173 1.56403 1.56736 1.58086

Alpha virt. eigenvalues -- 1.58150 1.59182 1.60050 1.60892 1.61401

Alpha virt. eigenvalues -- 1.61946 1.62438 1.62736 1.63521 1.64335

Alpha virt. eigenvalues -- 1.64656 1.65068 1.65538 1.65878 1.66749

Alpha virt. eigenvalues -- 1.66876 1.66960 1.68726 1.69158 1.70006

Alpha virt. eigenvalues -- 1.70203 1.70269 1.71531 1.72098 1.72526

Alpha virt. eigenvalues -- 1.73420 1.73464 1.73626 1.74617 1.75615

Alpha virt. eigenvalues -- 1.76345 1.77228 1.78325 1.78480 1.78783

Alpha virt. eigenvalues -- 1.79111 1.80525 1.81229 1.82087 1.82489

Alpha virt. eigenvalues -- 1.84342 1.84367 1.84856 1.85772 1.86124

Alpha virt. eigenvalues -- 1.86629 1.86891 1.87179 1.88647 1.88678

Alpha virt. eigenvalues -- 1.88920 1.89731 1.90274 1.90338 1.90448

Alpha virt. eigenvalues -- 1.92092 1.92566 1.93734 1.95271 1.95373

Alpha virt. eigenvalues -- 1.95880 1.96680 1.97169 1.97442 1.98857

Alpha virt. eigenvalues -- 1.99518 1.99722 2.00893 2.00912 2.01356

Alpha virt. eigenvalues -- 2.01804 2.02340 2.02830 2.03140 2.03516

Alpha virt. eigenvalues -- 2.03719 2.05009 2.06474 2.06809 2.07150

Alpha virt. eigenvalues -- 2.07266 2.08153 2.08980 2.09046 2.09966

Alpha virt. eigenvalues -- 2.10699 2.10994 2.11487 2.12129 2.14700

Alpha virt. eigenvalues -- 2.14782 2.14867 2.16074 2.17953 2.19011

Alpha virt. eigenvalues -- 2.19299 2.19813 2.20198 2.20874 2.22426

Alpha virt. eigenvalues -- 2.22792 2.23787 2.24753 2.25100 2.27292

Alpha virt. eigenvalues -- 2.27323 2.27936 2.28389 2.29359 2.29546

Alpha virt. eigenvalues -- 2.30875 2.31194 2.31551 2.33261 2.34775

Alpha virt. eigenvalues -- 2.36896 2.37007 2.37505 2.38136 2.38382

Alpha virt. eigenvalues -- 2.40863 2.40928 2.41979 2.42394 2.42487

Alpha virt. eigenvalues -- 2.43845 2.44714 2.44720 2.45852 2.46035

Alpha virt. eigenvalues -- 2.47865 2.50321 2.51371 2.51456 2.52146

Alpha virt. eigenvalues -- 2.52471 2.52731 2.53713 2.56396 2.58046

Alpha virt. eigenvalues -- 2.58491 2.58972 2.59683 2.59702 2.59910

Alpha virt. eigenvalues -- 2.60158 2.61601 2.63720 2.64936 2.66089

Alpha virt. eigenvalues -- 2.67592 2.68393 2.70063 2.70610 2.71040

Alpha virt. eigenvalues -- 2.71382 2.74246 2.75000 2.76167 2.77335

Alpha virt. eigenvalues -- 2.78566 2.80133 2.80163 2.82083 2.82118

Alpha virt. eigenvalues -- 2.83631 2.84621 2.85343 2.87614 2.89551

Alpha virt. eigenvalues -- 2.91280 2.91303 2.92987 2.95669 2.96089

Alpha virt. eigenvalues -- 2.97266 2.98507 2.98995 2.99741 3.01318

Alpha virt. eigenvalues -- 3.01952 3.02163 3.02294 3.04713 3.05649

Alpha virt. eigenvalues -- 3.06036 3.06395 3.07189 3.08757 3.09254

Alpha virt. eigenvalues -- 3.12170 3.12186 3.14359 3.14869 3.15178

Alpha virt. eigenvalues -- 3.15761 3.16199 3.16244 3.17822 3.18174

Alpha virt. eigenvalues -- 3.20188 3.20585 3.20646 3.21034 3.21640

Alpha virt. eigenvalues -- 3.21682 3.23117 3.23162 3.24685 3.24755

Alpha virt. eigenvalues -- 3.25803 3.26483 3.27480 3.28116 3.28662

Alpha virt. eigenvalues -- 3.29140 3.30328 3.31491 3.32679 3.33039

Alpha virt. eigenvalues -- 3.34492 3.35004 3.35301 3.36114 3.36170

Alpha virt. eigenvalues -- 3.36641 3.37174 3.38359 3.38762 3.39310

Alpha virt. eigenvalues -- 3.39417 3.40283 3.40693 3.41574 3.41860

Alpha virt. eigenvalues -- 3.42106 3.45704 3.45878 3.46041 3.46573

Alpha virt. eigenvalues -- 3.47205 3.47903 3.48576 3.49317 3.49568

Alpha virt. eigenvalues -- 3.49606 3.50629 3.50782 3.52336 3.52768

Alpha virt. eigenvalues -- 3.53368 3.55420 3.56157 3.56977 3.57853

Alpha virt. eigenvalues -- 3.59032 3.60486 3.60995 3.61261 3.61541

Alpha virt. eigenvalues -- 3.62013 3.62054 3.63789 3.63801 3.64315

Alpha virt. eigenvalues -- 3.64448 3.65922 3.67344 3.67601 3.67762

Alpha virt. eigenvalues -- 3.68270 3.69151 3.69259 3.70603 3.72115

Alpha virt. eigenvalues -- 3.72303 3.72778 3.74476 3.74704 3.75800

Alpha virt. eigenvalues -- 3.76295 3.76815 3.77192 3.78293 3.78609

Alpha virt. eigenvalues -- 3.79711 3.80457 3.81055 3.81553 3.82100

Alpha virt. eigenvalues -- 3.82780 3.83777 3.84846 3.86656 3.86903

Alpha virt. eigenvalues -- 3.87001 3.87610 3.87710 3.88904 3.90203

Alpha virt. eigenvalues -- 3.91897 3.92335 3.93390 3.94816 3.95332

Alpha virt. eigenvalues -- 3.95680 3.95949 3.97689 3.98370 3.98382

Alpha virt. eigenvalues -- 4.00047 4.00875 4.02225 4.02597 4.02774

Alpha virt. eigenvalues -- 4.03179 4.04237 4.05608 4.06368 4.06828

Alpha virt. eigenvalues -- 4.07237 4.08279 4.08441 4.08706 4.09313

Alpha virt. eigenvalues -- 4.11750 4.11863 4.12256 4.13294 4.13630

Alpha virt. eigenvalues -- 4.13784 4.14276 4.15417 4.16607 4.17014

Alpha virt. eigenvalues -- 4.18184 4.18961 4.19000 4.20146 4.20824

Alpha virt. eigenvalues -- 4.20931 4.21088 4.21176 4.22665 4.23154

Alpha virt. eigenvalues -- 4.24143 4.24747 4.25809 4.26343 4.28062

Alpha virt. eigenvalues -- 4.28274 4.28810 4.28965 4.29680 4.33990

Alpha virt. eigenvalues -- 4.34474 4.34636 4.34820 4.35845 4.37428

Alpha virt. eigenvalues -- 4.37840 4.38144 4.38546 4.39763 4.41767

Alpha virt. eigenvalues -- 4.41962 4.42173 4.43071 4.43284 4.46268

Alpha virt. eigenvalues -- 4.47219 4.48199 4.48226 4.49541 4.49732

Alpha virt. eigenvalues -- 4.49918 4.50166 4.51262 4.52006 4.52303

Alpha virt. eigenvalues -- 4.53582 4.54783 4.54975 4.56867 4.57338

Alpha virt. eigenvalues -- 4.58658 4.59217 4.59233 4.60718 4.60953

Alpha virt. eigenvalues -- 4.62286 4.65100 4.66880 4.68959 4.69291

Alpha virt. eigenvalues -- 4.70831 4.72420 4.73516 4.76085 4.76358

Alpha virt. eigenvalues -- 4.76598 4.76901 4.77434 4.77897 4.79155

Alpha virt. eigenvalues -- 4.80231 4.83380 4.84344 4.84861 4.85112

Alpha virt. eigenvalues -- 4.88039 4.88373 4.89090 4.89892 4.90232

Alpha virt. eigenvalues -- 4.90360 4.92298 4.93784 4.94036 4.94311

Alpha virt. eigenvalues -- 4.97108 4.97677 4.99223 4.99867 5.01279

Alpha virt. eigenvalues -- 5.01405 5.02583 5.03347 5.04048 5.04762

Alpha virt. eigenvalues -- 5.06206 5.06277 5.08145 5.09982 5.13104

Alpha virt. eigenvalues -- 5.13134 5.13331 5.15639 5.15911 5.18517

Alpha virt. eigenvalues -- 5.18868 5.20631 5.22594 5.26329 5.26876

Alpha virt. eigenvalues -- 5.28971 5.30680 5.35202 5.37096 5.38646

Alpha virt. eigenvalues -- 5.39243 5.42078 5.44802 5.45573 5.47025

Alpha virt. eigenvalues -- 5.48903 5.51632 5.51832 5.54021 5.57791

Alpha virt. eigenvalues -- 5.64827 5.67062 5.71887 5.75453 5.75753

Alpha virt. eigenvalues -- 5.76067 5.76796 5.82132 5.84395 5.88047

Alpha virt. eigenvalues -- 5.90661 5.92038 5.96972 5.98480 6.00497

Alpha virt. eigenvalues -- 6.04127 6.07073 6.08511 6.09637 6.13404

Alpha virt. eigenvalues -- 6.13967 6.16452 6.17811 6.22156 6.24049

Alpha virt. eigenvalues -- 6.27671 6.28402 6.37479 6.39373 6.42797

Alpha virt. eigenvalues -- 6.46305 6.48323 6.50014 6.52001 6.52266

Alpha virt. eigenvalues -- 6.55685 6.63368 6.64428 6.64524 6.64767

Alpha virt. eigenvalues -- 6.67007 6.67709 6.68151 6.68528 6.73623

Alpha virt. eigenvalues -- 6.81124 6.84637 6.85481 6.94168 6.94899

Alpha virt. eigenvalues -- 7.00178 7.05156 7.06207 7.06662 7.07838

Alpha virt. eigenvalues -- 7.09767 7.15350 7.19838 7.25698 7.26144

Alpha virt. eigenvalues -- 7.27400 7.31783 7.38303 7.39587 7.47704

Alpha virt. eigenvalues -- 7.50970 7.70319 7.77253 7.81821 7.98593

Alpha virt. eigenvalues -- 8.07689 8.08623 8.34768 8.38325 14.85869

Alpha virt. eigenvalues -- 15.06957 15.49864 15.89220 16.05344 16.84250

Alpha virt. eigenvalues -- 16.89055 17.50696 18.55976 18.72266 19.06712

Alpha virt. eigenvalues -- 19.28418 19.80365 19.88715 20.31826 20.86672

Alpha virt. eigenvalues -- 21.14832

Normal termination of Gaussian 16