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

 9-Oct-2018

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

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

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 Standard orientation:

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 Center Atomic Atomic Coordinates (Angstroms)

 Number Number Type X Y Z

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 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

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 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:

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

 3500 cm-1 subtracted from the computed wavenumbers

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 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:

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 Numbering added /JS-L

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 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)

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 (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