

♠ https://bse.pnl.gov/bse/portal/user/anon/panel/Main/template/courier\_conten



## BASIS SET CHANGE

```
# 6-311G EMSL Basis Set Exchange Library 1/30/14 2:44 AM
# Elements
                                      References
± -----
                                       _____
# H, Li - Ne: R. Krishnan, J.S. Binkley, R. Seeger and J.A. Pople,
             J. Chem. Phys. 72, 650 (1980)
# Na - Ar: A.D. McLean and G.S. Chandler J. Chem. Phys. 72, 5639, (1980).
            J-P. Blaudeau, M. P. McGrath, L.A. Curtiss and L. Radom,
# K - Ca:
             J. Chem. Phys. 107, 5016 (1997).
# Ga - Kr: L. A. Curtiss, M. P. McGrath, J-P. Blandeau, N. E. Davis,
             R. C. Binning, Jr. L. Radom, J. Chem. Phys. 103, 6104 (1995).
            M.N. Glukhovstev, A. pross, M.P. McGrath, L. Radom, J. Chem. Phys.
             103, 1878 (1995)
BASIS "ao basis" PRINT
#BASIS SET: (11s,5p) -> [4s,3p]
Be
     S
  1682.8000000
                            0.00228574
   251.7150000
                            0.0175938
     57.4116000
                            0.0863315
     16.5171000
                            0.2818350
     4.8536400
                            0.6405940
     0.6268630
                            0.1444670
Be
     SP
     8.3093800
                           0.1086210
                                                    0.0361344
     1.7407500
                            0.9273010
                                                   0.2169580
     0.4858160
                           -0.00297169
                                                   0.8418390
     SP
Be
     0.1636130
                            1.0000000
                                                   1.0000000
     SP
Be
     0.0567285
                            1.0000000
                                                   1.0000000
END
```