

BASIS SET EXCHANGE

v1.2.2

```
# 3-21G EMSL Basis Set Exchange Library 1/30/14 2:40 AM
# Elements References
# -----
# H - Ne: J.S. Binkley, J.A. Pople, W.J. Hehre, J. Am. Chem. Soc 102 939 (1980)
# Na - Ar: M.S. Gordon, J.S. Binkley, J.A. Pople, W.J. Pietro and W.J. Hehre,
# J. Am. Chem. Soc. 104, 2797 (1983).
# K - Ca: K.D. Dobbs, W.J. Hehre, J. Comput. Chem. 7, 359 (1986).
# Ga - Kr: K.D. Dobbs, W.J. Hehre, J. Comput. Chem. 7, 359 (1986).
# Sc - Zn: K.D. Dobbs, W.J. Hehre, J. Comput. Chem. 8, 861 (1987).
# Y - Cd: K.D. Dobbs, W.J. Hehre, J. Comput. Chem. 8, 880 (1987).
# Cs : A 3-21G quality set derived from the Huzinaga MIDI basis sets.
# E.D. Glendening and D. Feller, J. Phys. Chem. 99, 3060 (1995)
#
```

```
BASIS "ao basis" PRINT
#BASIS SET: (3s) -> [2s]
H S
    5.4471780      0.1562850
    0.8245470      0.9046910
H S
    0.1831920      1.0000000
END
```