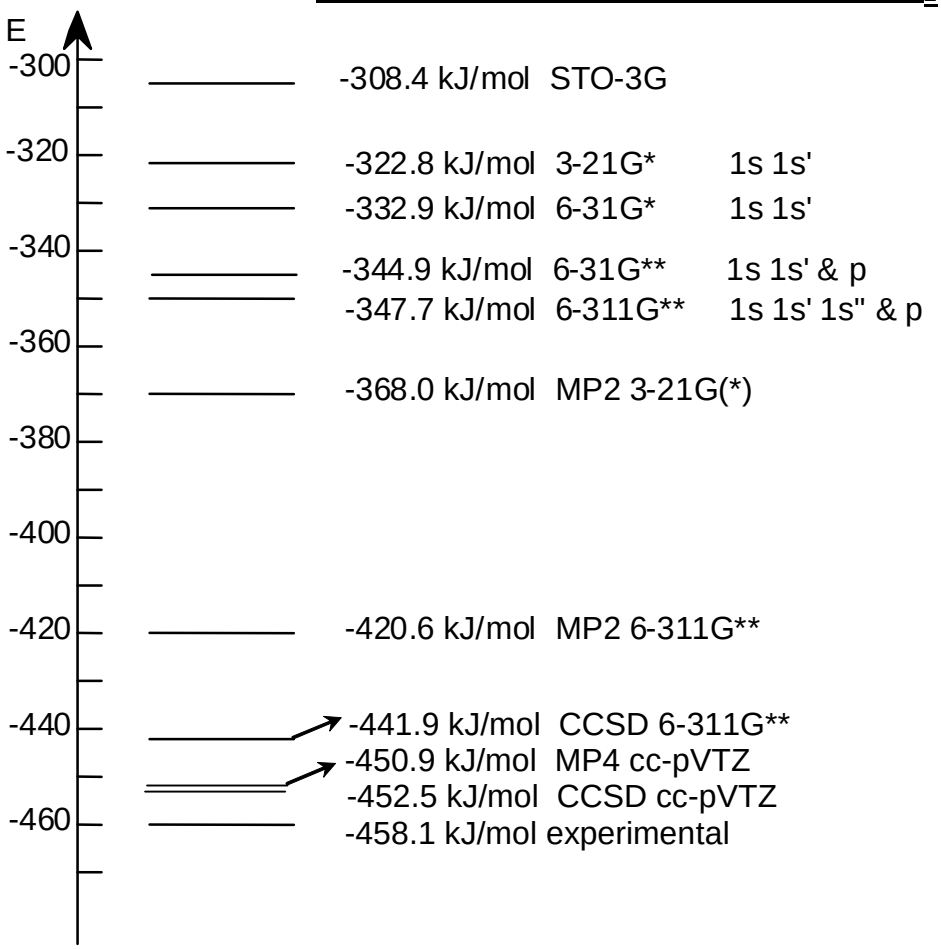
***Ab initio* Molecular Orbital Treatment for H_2**



Atomic Orbital Terms in Valence Shell (number of Gaussian primitives)

Atoms:	Hydrogen				1st and 2nd row						1st row	2nd row
Orbital:	1s	1s'	1s''	2p	s	s'	s''	p	p'	p''	3d	3d
STO-3G	3				3			3				
3-21G(*)	2	1			2	1		2	1			1
3-21G*	2	1			2	1		2	1		1	1
6-31G*	3	1			3	1		3	1		1	1
6-31G**	3	1		1	3	1		3	1		1	1
6-311G**	3	1	1	1	3	1	1	3	1	1	1	1
cc-pVTZ	7	1	1	2p1d	7	1	1	3	1	1	2d1f	2d1f

cc-pVTZ gaussian coefficients (α) different for valence s(7-711) and p(7-311) orbitals.

Note: A 6-31G* or 6-31G** orbital uses 6 total primitives for a core orbital and 5 total primitives for a valence s or p orbital

H_2 at 6-311G** :

$$\Psi_{MO} = 0.186\ 1S_A(\text{inner}) + 0.288\ 1S_A(\text{middle}) + 0.133\ 1S_A(\text{outer}) + 0.023\ 2P_{ZA} + 0.186\ 1S_B(\text{inner}) + 0.288\ 1S_B(\text{middle}) + 0.133\ 1S_B(\text{outer}) - 0.023\ 2P_{ZB}$$

W.J. Hehre, L.Radom, P. v.R. Schlyer, J.A.Pople, *Ab Initio Molecular Orbital Theory,* Wiley, New York, NY, **1986**