

HOMONUCLEAR DIATOMIC MOLECULES

MOLECULE	ELECTRON CONFIGURATION	BOND ORDER	D_e/eV	$R_e/\text{\AA}$
H_2^+	$1\sigma_g \quad 2\Sigma_g^+$	0.5	2.79	1.06
H_2	$1\sigma_g^2 \quad 1\Sigma_g^+$	1	4.75	0.741
He_2	$1\sigma_g^2 1\sigma_u^2 \quad 1\Sigma_g^+$	0	0.0009 [1]	3.0
	$1\sigma_g^2 1\sigma_u 2\sigma_g \quad 3\Sigma_u^+ \quad [2]$	1	2.6	1.05
He_2^+	$1\sigma_g^2 1\sigma_u \quad 2\Sigma_u^+$	0.5	2.5	1.08
Li_2	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 \quad 1\Sigma_g^+$	1	1.07	2.67
Be_2	$1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 \quad 1\Sigma_g^+$	0	0.1	2.5
B_2	$\dots 1\pi_u^2 \quad 3\Sigma_g^- \quad [3]$	1	3.0	1.59
C_2	$\dots 1\pi_u^4 \quad 1\Sigma_g^+$	2	6.3	1.24
N_2	$\dots 1\pi_u^4 3\sigma_g^2 \quad 1\Sigma_g^+$	3	9.91	1.10
N_2^+	$\dots 1\pi_u^4 3\sigma_g \quad 2\Sigma_g^+$	2.5	8.85 [4]	1.12
O_2	$\dots 3\sigma_g^2 1\pi_u^4 1\pi_g^2 \quad 3\Sigma_g^- \quad [3, 5]$	2	5.21	1.21
O_2^+	$\dots 3\sigma_g^2 1\pi_u^4 1\pi_g \quad 2\Pi_g$	2.5	6.78 [4]	1.12
F_2	$\dots 1\pi_u^4 3\sigma_g^2 1\pi_g^4 \quad 1\Sigma_g^+$	1	1.66	1.41
Ne_2	$\dots 1\pi_u^4 3\sigma_g^2 1\pi_g^4 3\sigma_u^2 \quad 1\Sigma_g^+$	0	0.0036 [1]	3.1

NOTES:

[1] Van der Waals bonding.

[2] Lifetime $\approx 10^{-4}$ sec.

[3] Note application of Hund's rules.

[4] Compare effects of ionization on relative binding energies for N_2^+ and O_2^+ .

[5] Paramagnetism of O_2 predicted by MO theory.