

Table 6.1 Energies and 'coefficients' of 1,3-dipoles

Dipole	HOMO		LUMO	
	Energy (eV)	$(c\beta)^2/15$	Energy (eV)	$(c\beta)^2/15$
Nitrile ylids	-7.7	$\text{CH}\equiv\overset{+}{\text{N}}-\overset{-}{\text{CH}}_2$ 1.07 1.50	0.9	$\text{CH}\equiv\overset{+}{\text{N}}-\overset{-}{\text{CH}}_2$ 0.69 0.64
PhC $\equiv\overset{+}{\text{N}}-\overset{-}{\text{CH}}_2$	-6.4		0.6	
Nitrile imines	-9.2	$\text{CH}\equiv\overset{+}{\text{N}}-\overset{-}{\text{NH}}$ 0.90 1.45	0.1	$\text{CH}\equiv\overset{+}{\text{N}}-\overset{-}{\text{NH}}$ 0.92 0.36
PhC $\equiv\overset{+}{\text{N}}-\overset{-}{\text{NH}}$	-7.5		-0.5	
Nitrile oxides	-11.0	$\text{CH}\equiv\overset{+}{\text{N}}-\overset{-}{\text{O}}$ 0.81 1.24	-0.5	$\text{CH}\equiv\overset{+}{\text{N}}-\overset{-}{\text{O}}$ 1.18 0.17
PhC $\equiv\overset{+}{\text{N}}-\overset{-}{\text{O}}$	-10.0		-1.0	
Diazoalkanes	-9.0	$\text{CH}_2=\overset{+}{\text{N}}=\overset{-}{\text{N}}$ 1.57 0.85	1.8	$\text{CH}_2=\overset{+}{\text{N}}=\overset{-}{\text{N}}$ 0.66 0.56
Azides	-11.5	$\text{HN}=\overset{+}{\text{N}}=\overset{-}{\text{N}}$ 1.55 0.72	0.1	$\text{HN}=\overset{+}{\text{N}}=\overset{-}{\text{N}}$ 0.37 0.76
PhN $=\overset{+}{\text{N}}=\overset{-}{\text{N}}$	-9.5		-0.2	
Nitrous oxide	-12.9	$\text{N}\equiv\overset{+}{\text{N}}-\overset{-}{\text{O}}$ 0.67 1.33	-1.1	$\text{N}\equiv\overset{+}{\text{N}}-\overset{-}{\text{O}}$ 0.96 0.19
Azomethine ylids	-6.9	$\text{CH}_2=\overset{+}{\text{N}}(\text{H})-\overset{-}{\text{CH}}_2$ 1.28 1.28	1.4	$\text{CH}_2=\overset{+}{\text{N}}(\text{H})-\overset{-}{\text{CH}}_2$ 0.73 0.73
Ar N ⁺ RO ₂ CCH= N ⁺ - CHCO ₂ R	-7.7		-0.6	
Azomethine imines	-8.6	$\text{CH}_2=\overset{+}{\text{N}}(\text{H})-\overset{-}{\text{NH}}$ 1.15 1.24	-0.3	$\text{CH}_2=\overset{+}{\text{N}}(\text{H})-\overset{-}{\text{NH}}$ 0.87 0.49
PhCH= N ⁺ - NPh	-5.6		-1.4	
CH ₂ = N ⁺ - NCOR	-9.0		-0.4	
Nitrones	-9.7	$\text{CH}_2=\overset{+}{\text{N}}(\text{H})-\overset{-}{\text{O}}$ 1.11 1.06	-0.5	$\text{CH}_2=\overset{+}{\text{N}}(\text{H})-\overset{-}{\text{O}}$ 0.98 0.32
R N ⁺ CH ₂ = N ⁺ - O ⁻	-8.7		0.3	
PhCH= N ⁺ - O ⁻	-8.0		-0.4	
Carbonyl ylids	-7.1	$\text{CH}_2=\overset{+}{\text{O}}-\overset{-}{\text{CH}}_2$ 1.29 1.29	0.4	$\text{CH}_2=\overset{+}{\text{O}}-\overset{-}{\text{CH}}_2$ 0.82 0.82
Ar(NC)C= O ⁺ - C ⁻ (CN)Ar	-6.5		-0.6	
(NC) ₂ C= O ⁺ - C ⁻ (CN) ₂	-9.0		-1.1	
Carbonyl imines	-8.6	$\text{CH}_2=\overset{+}{\text{O}}-\overset{-}{\text{NH}}$ 1.04 1.34	-0.2	$\text{CH}_2=\overset{+}{\text{O}}-\overset{-}{\text{NH}}$ 1.06 0.49
Carbonyl oxides	-10.3	$\text{CH}_2=\overset{+}{\text{O}}-\overset{-}{\text{O}}$ 0.82 1.25	-0.9	$\text{CH}_2=\overset{+}{\text{O}}-\overset{-}{\text{O}}$ 1.30 0.24
Ozone	-13.5		-2.2	