

Properties of Common Organic Materials

	Unit	Alq ₃	Anthracene	C ₆₀	CuPc	Pentacene	Ir(ppy) ₃	PTCDA
Chemical formula		C ₂₇ H ₁₈ AlN ₃ O ₃	C ₁₄ H ₁₀	C ₆₀	C ₃₂ H ₁₆ CuN ₈	C ₂₂ H ₁₄	C ₃₃ H ₂₄ IrN ₃	C ₂₄ H ₈ O ₆
Density	g/cm ³	1.31	1.24	1.62	1.98	1.3	1.73	1.7
Energy gap ^(a)	eV	2.77	3.59	3.55	2.03	2.1	3.41	2.2
Molecular weight	gm/M	459.4	178.2	720.6	576.1	278.4	654.8	392.3
Rel. dielectric constant		3.5	2.35	4.08	3.6	4.0	2.9	3.6
Crystal structure		triclinic	monoclinic	fcc	triclinic	triclinic	triclinic	monoclinic
Crystal space group		$P\bar{1}$	$P2_1 / b$	$Fm\bar{3}m$	$P\bar{1}$	$P\bar{1}$	$P\bar{3}$	$P2_1 / c$
Crystal point group ^(b)		C ₃ (<i>f</i>), C ₁ (<i>m</i>)	D _{2h} ⁵	I _h	D _{4h}	D _{2h}	C ₃ (<i>f</i>), C ₁ (<i>m</i>)	2/ <i>m</i>

(a) Nominally quoted as the energy of the π - π^* transition, or HOMO-LUMO gap

(b) *f*=facial, *m*=meridonal isomers