

IR Material Selection Guide

Use this guide to help determine the best IR materials for certain applications. The guide provides information on several materials' transmission range, water solubility, and refractive index. Also included are recommended cleaning agents, solvents to avoid, reactivity with the sample, mechanical, and thermal characteristics.

If a material is hygroscopic (absorbs moisture from the air), it is so noted in the Remarks column. Hygroscopic materials are used most frequently with organic compounds. Nonhygroscopic materials are typically used for samples containing water. Materials with a higher refractive index (such as KRS-5, Ge, ZnS, and ZnSe) are usually used as internal reflection elements in ATR accessories.

Material	Transmission Range (cm ⁻¹)	Useful Range for ATR (cm ⁻¹)	Refractive Index @1000 cm ⁻¹	%Trans. (window thickness)	Remarks
NaCl	40000 – 625	N/A	1.49	91.5 (4 mm)	hygroscopic, withstands thermal & mechanical shock
KBr	40000 – 400	N/A	1.52	90.5 (4 mm)	hygroscopic, withstands thermal & mechanical shock
CsI	40000 – 200	N/A	1.74	92 (2 mm)	hygroscopic, easily scratched, soft
CaF ₂	50000 – 1111	N/A	1.39	90 (4 mm)	withstands high pressure, resists most acids & bases
BaF ₂	50000 – 740	N/A	1.42	90 (3 mm)	subject to thermal & mechanical shock
AgCl	25000 – 360	N/A	1.98	84 (3 mm)	cold flows, attacks base metals, sensitive to UV
ZnS	17000 – 720	17000 – 950	2.2	70 (1 mm)	good ATR material, withstands shock
Sapphire	50000 – 1600	50000 – 1780	1.74	70 (2 mm)	hard, inert
AMTIR	11000 – 625	11000 – 840	2.5	68 (2 mm)	relatively hard, brittle, good ATR material
Ge	5500 – 475	5500 – 675	4.0	50 (2 mm)	hard & brittle, good ATR material, temp. sensitive
ZnSe	20000 – 454	20000 – 650	2.4	65 (1 mm)	hard & brittle, good ATR material
Si	8300 – 660 & 360 – 70	8300 – 1500 & 360 – 120	3.4	55 (2.5 mm)	hard & brittle, withstands thermal shock, inert
CdTe	20000 – 360	N/A	2.67	40 (5 mm)	very brittle, easily cracked
Diamond	4500 – 2500 & 1667 – 33	4200 – 200	2.4	70 (1 mm)	very hard, withstands high pressure, chemically inert
KRS-5	20000 – 250	20000 – 400	2.37	70 (2 mm)	deforms under pressure, conventional ATR material
Quartz	25000 – 2200	N/A	1.4	90 (3mm)	hard, inert

Material	Water Sol. (g/100g H ₂ O) @25°C	Max. useful temp. in air (°C)	Density g/cm ³	Cleaning Agents	Solvents which attack material	Hardness (Knoop#)
NaCl	35.7	400	2.17	anhydrous solvents	lower alcohols "wet" solvents	15
KBr	53.5	300	2.75	anhydrous solvents	lower alcohols "wet" solvents	7
CsI	44.4	200	4.50	anhydrous solvents	lower alcohols "wet" solvents	20
CaF ₂	0.0013	900	3.18	acetone, alcohol	NH ₄ ⁺ salts, acids	158
BaF ₂	0.17	500	4.83	acetone, alcohol	NH ₄ ⁺ salts, acids	82
AgCl	0.00015	200	6.47	acetone, CH ₂ Cl ₂	complexing agents*	9.5
ZnS	0.00069	300	4.08	acetone, alcohol	acids	178
Sapphire	insol.	1700	4.00	alcohol, acetone, H ₂ O	acids, alkalies	1370
AMTIR	insol.	300	4.40	alcohol, acetone, H ₂ O	alkalies	170
Ge	insol.	270	5.32	alcohol, acetone, H ₂ O	H ₂ SO ₄ , aqua regia	550
ZnSe	insol.	300	5.27	alcohol, acetone, H ₂ O	acids, strong alkalies	137
Si	insol.	300	2.33	alcohol, acetone, H ₂ O	HF, HNO ₃	1150
CdTe	insol.	300	6.2	alcohol, acetone	acids, HNO ₃	56
Diamond	insol.	750	3.51	alcohol, acetone	K ₂ Cr ₂ O ₇ , conc. H ₂ SO ₄	7000
KRS-5	0.05	200	7.37	MEK	complexing agents*	40
Quartz	insol.	1200	2.203	alcohol, acetone, H ₂ O	HF, some hot acids and bases	820

* Typical complexing agents include ammonium salts & materials such as EDTA.

