



**ANALYTICAL**

**LIFE SCIENCE**

**PROCESS**

# GUIDE

## for Infrared Spectroscopy



[www.brukeroptics.com](http://www.brukeroptics.com)

## IR-Spectroscopy

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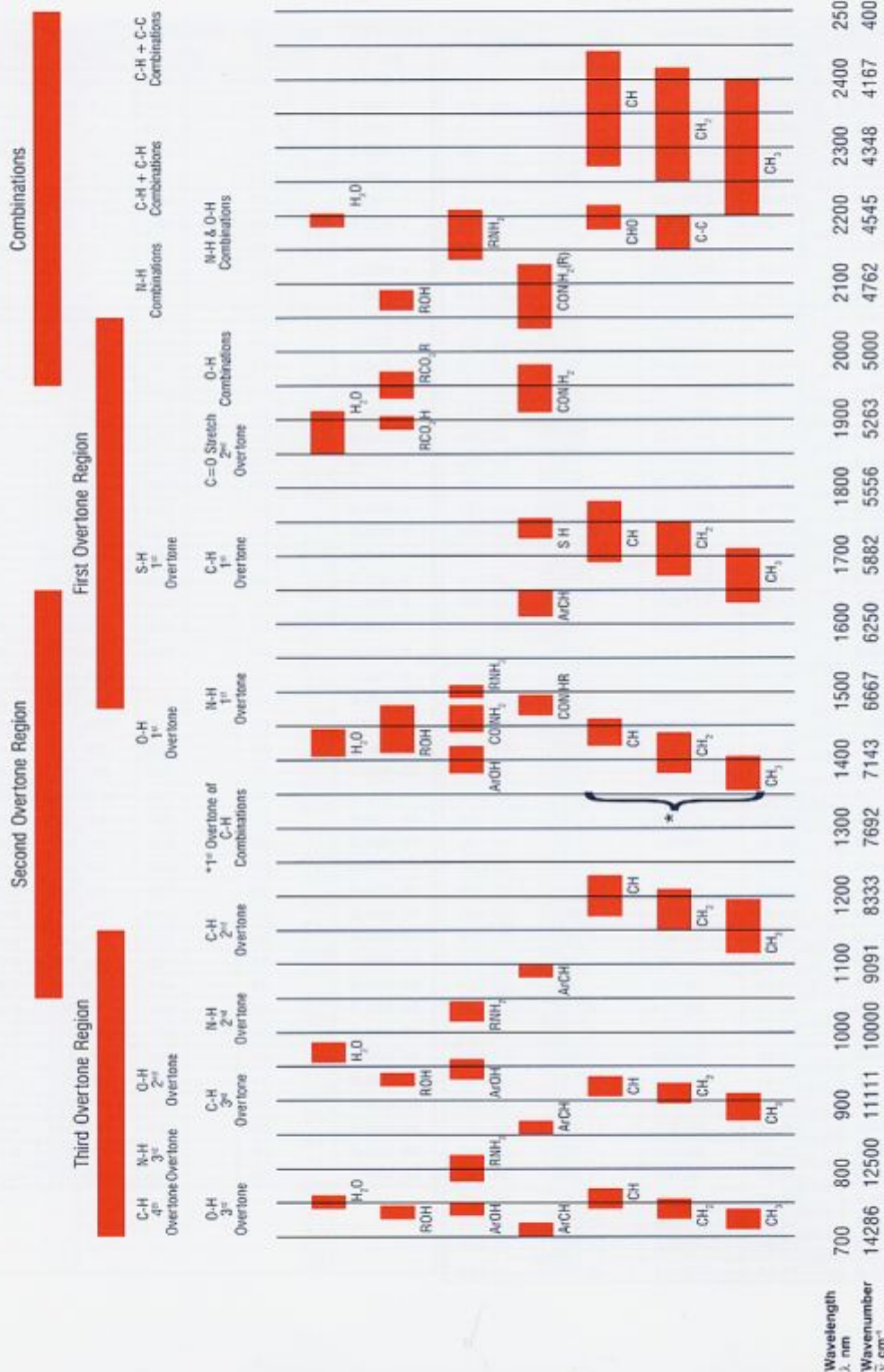
## Conversion Table of Energy and Wavelength Units

Wavenumber [cm <sup>-1</sup> ]	Wavelength [Micron]	Wavelength [nm]	Frequency [GHz]	Electron Volt [eV]	Wavenumber [cm <sup>-1</sup> ]	Wavelength [Micron]	Wavelength [nm]	Frequency [GHz]	Electron Volt [eV]
2.0	5 000.00	5 0000 00	60	.00 025	1 000.0	10.00	10 000	29 979	.12 398
4.0	2 500.00	2 500 000	120	.00 050	1 100.0	9.09	9 091	32 977	.13 638
6.0	1 666.67	1 666 667	180	.00 074	1 200.0	8.33	8 333	35 975	.14 878
8.0	1 250.00	1 250 000	240	.00 099	1 300.0	7.69	7 692	38 973	.16 118
10.0	1 000.00	1 000 000	300	.00 124	1 400.0	7.14	7 143	41 971	.17 358
12.0	833.33	833 333	360	.00 149	1 500.0	6.67	6 667	44 968	.18 598
14.0	714.29	714 286	420	.00 174	1 600.0	6.25	6 250	47 966	.19 837
16.0	625.00	625 000	480	.00 198	1 700.0	5.88	5 882	50 964	.21 077
18.0	555.56	555 556	540	.00 223	1 800.0	5.56	5 556	53 962	.22 317
20.0	500.00	500 000	600	.00 248	1 900.0	5.26	5 263	56 960	.23 557
22.0	454.55	454 545	660	.00 273	2 000.0	5.00	5 000	59 958	.24 797
24.0	416.57	416 667	719	.00 298	2 200.0	4.55	4 545	65 954	.27 276
26.0	384.62	384 615	779	.00 322	2 400.0	4.17	4 167	71 950	.29 756
28.0	357.14	357 143	839	.00 347	2 600.0	3.85	3 846	77 945	.32 236
30.0	333.33	333 333	898	.00 372	2 800.0	3.57	3 571	83 941	.34 716
32.0	312.50	312 500	959	.00 397	3 000.0	3.33	3 333	89 937	.37 195
34.0	294.12	294 118	1 019	.00 422	3 200.0	3.13	3 125	95 933	.39 675
36.0	277.78	277 778	1 079	.00 446	3 400.0	2.94	2 941	101 929	.42 155
38.0	263.16	263 158	1 139	.00 471	3 600.0	2.78	2 778	107 924	.44 634
40.0	250.00	250 000	1 199	.00 496	3 800.0	2.63	2 632	113 920	.47 114
50.0	200.00	200 000	1 499	.00 620	4 000.0	2.50	2 500	119 916	.49 594
60.0	166.67	166 667	1 799	.00 744	5 000.0	2.00	2 000	149 895	.61 992
70.0	142.86	142 857	2 099	.00 868	6 000.0	1.67	1 667	179 874	.74 390
80.0	125.00	125 000	2 398	.00 992	7 000.0	1.43	1 429	209 853	.86 789
90.0	111.11	111 111	2 698	.01 116	8 000.0	1.25	1 250	239 832	.99 187
100.0	100.00	100 000	2 988	.01 240	9 000.0	1.11	1 111	269 811	1.11 586
110.0	90.91	90 909	3 298	.01 364	10 000.0	1.00	1 000	299 790	1.23 984
120.0	83.33	83 333	3 597	.01 488	11 000.0	.91	909	329 769	1.36 382
130.0	76.92	76 923	3 897	.01 612	12 000.0	.83	833	359 748	1.48 781
140.0	71.43	71 429	4 197	.01 736	13 000.0	.77	769	389 727	1.61 179
150.0	66.67	66 667	4 497	.01 860	14 000.0	.71	714	419 706	1.73 578
160.0	62.50	62 500	4 797	.01 984	15 000.0	.67	667	449 685	1.85 976
170.0	58.82	58 824	5 096	.02 108	16 000.0	.62	625	479 664	1.98 374
180.0	55.56	55 556	5 396	.02 232	17 000.0	.59	588	509 643	2.10 773
190.0	52.63	52 632	5 696	.02 356	18 000.0	.56	556	539 622	2.23 171
200.0	50.00	50 000	5 996	.02 480	19 000.0	.53	526	569 601	2.35 570
220.0	45.45	45 455	6 595	.02 728	20 000.0	.50	500	599 580	2.47 968
240.0	41.67	41 667	7 195	.02 976	22 000.0	.45	455	659 538	2.72 765
260.0	38.46	38 462	7 795	.03 224	24 000.0	.42	417	719 496	2.97 562
280.0	35.71	35 714	8 394	.03 472	26 000.0	.38	385	779 454	3.22 358
300.0	33.33	33 333	8 994	.03 720	28 000.0	.36	357	839 412	3.47 155
320.0	31.25	31 250	9 593	.03 967	30 000.0	.33	333	899 370	3.71 952
340.0	29.41	29 412	10 193	.04 215	32 000.0	.31	312	959 328	3.96 749
360.0	27.78	27 778	10 792	.04 463	34 000.0	.29	294	1 019 286	4.21 546
380.0	26.32	26 316	11 392	.04 711	36 000.0	.28	278	1 079 244	4.46 342
400.0	25.00	25 000	11 992	.04 959	38 000.0	.26	263	1 139 202	4.71 139
500.0	20.00	20 000	14 990	.06 199	40 000.0	.25	250	1 199 160	4.95 936
600.0	16.67	16 667	17 987	.07 439					
700.0	14.29	14 286	20 985	.08 679					
800.0	12.50	12 500	23 983	.09 919					
900.0	11.11	11 111	26 981	.11 159					

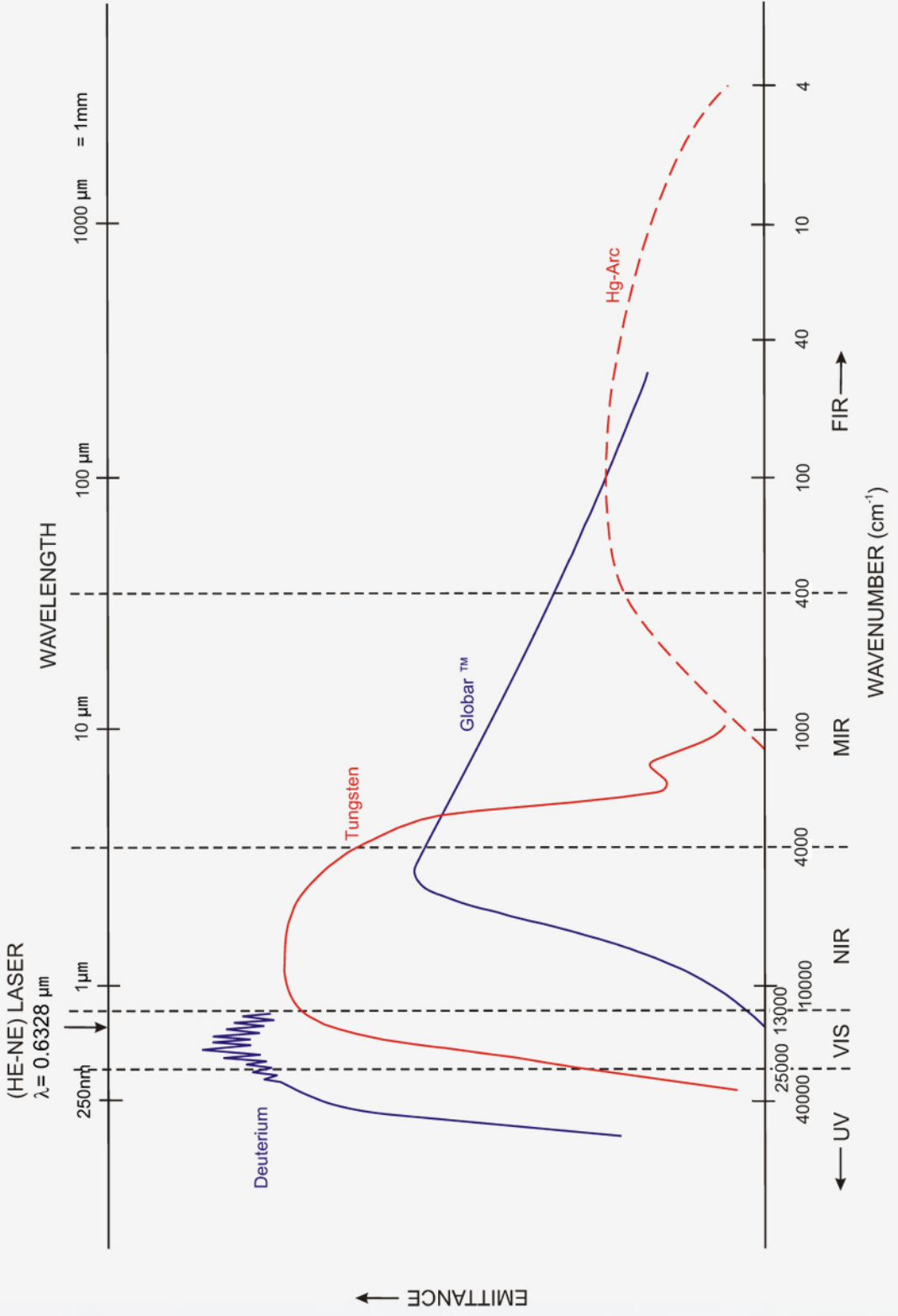
# Near Infrared Table



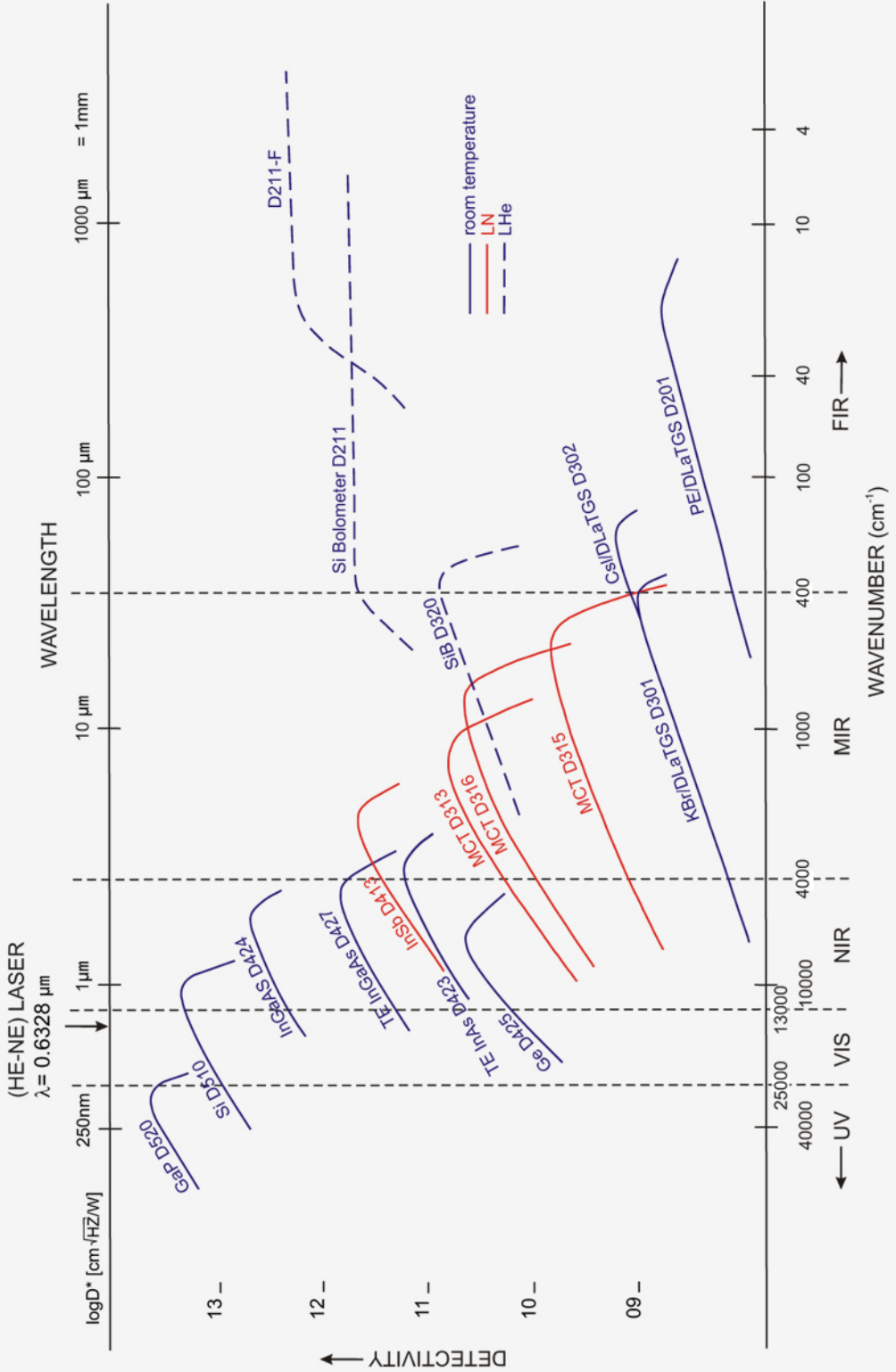
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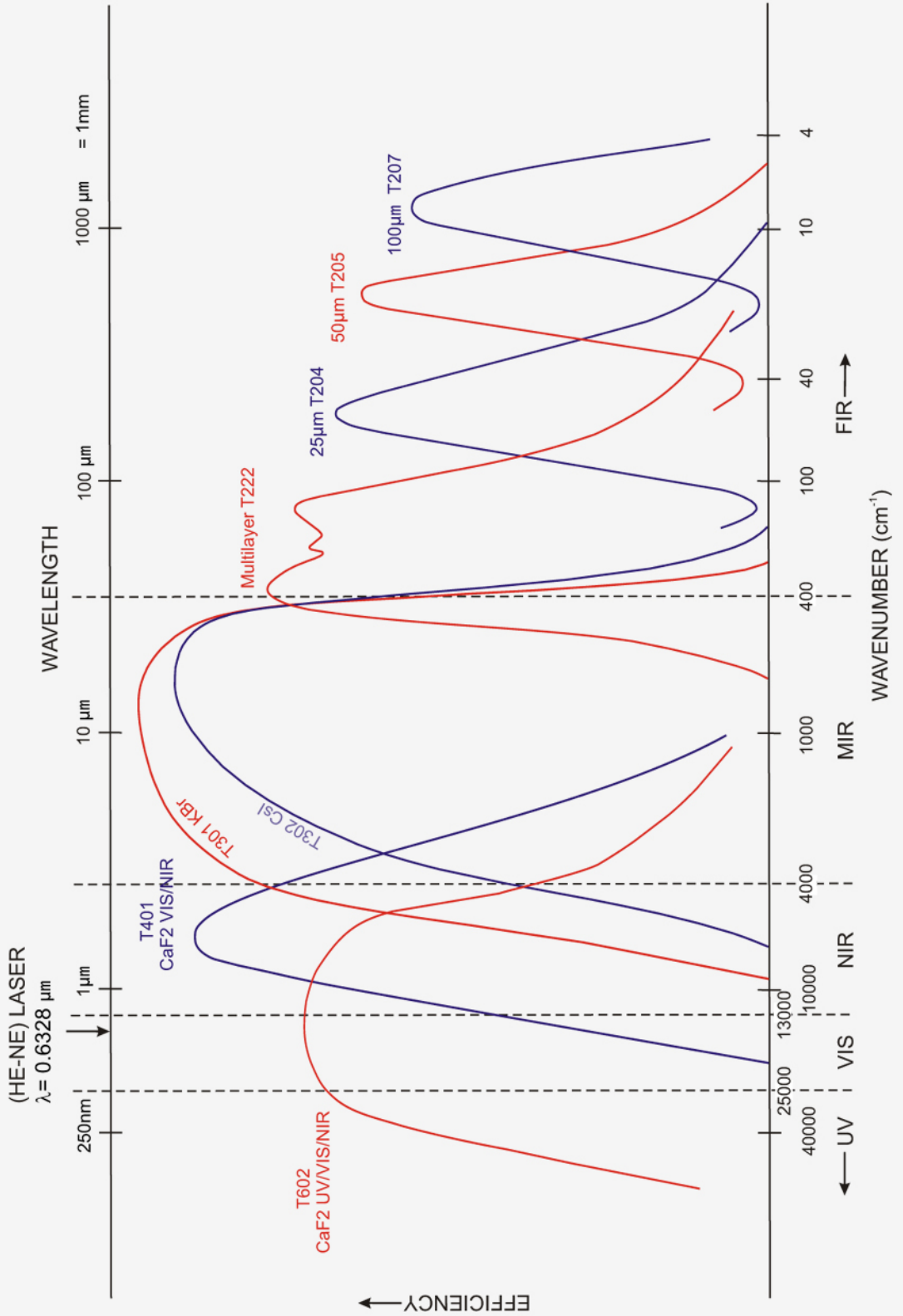
## SOURCES



## DETECTORS



## BEAMSPLITTERS



Material	Transmission Range [cm <sup>-1</sup> ] ([micrometers])	Refractive Index n at 2000 cm <sup>-1</sup>	Reflectance loss per surface	Hardness (Knoop)	Chemical Properties
Infrasil SiO <sub>2</sub>	57,000-2,800 (0.175-3.6)	1.46	~ 3.3 %	461	Insoluble in water; soluble in HF.
UV Sapphire Al <sub>2</sub> O <sub>3</sub>	66,000-2,000 (0.15-5.0)	1.75	~ 7.3 %	1370	Very slightly soluble in acids and bases.
Silicon Si	10,000-100 (1.0-100)	3.42	~ 30 %	1150	Insoluble in most acids and bases; soluble in HF and HNO <sub>3</sub> .
Calcium Fluoride CaF <sub>2</sub>	66,000-1,200 (0.15-8.0)	1.40	~ 2.8%	158	Insoluble in water; resists most acids and bases; soluble in NH <sub>4</sub> salts.
Barium Fluoride BaF <sub>2</sub>	50,000-900 (0.2-11)	1.45	~ 3.3%	82	Low water solubility; soluble in acid and NH <sub>4</sub> Cl.
Zinc Sulfide, Cleartran ZnS	22,000-750 (0.45-13.0)	2.25	~ 15%	355	Soluble in acid; insoluble in water.
Germanium Ge	5,000-600 (2.0-17)	4.01	~ 36%	550	Insoluble in water; soluble in hot H <sub>2</sub> SO <sub>4</sub> and aqua regia.
Sodium Chloride NaCl	28,000-700 (0.35-15)	1.52	~ 4.5%	15	Hygroscopic; slightly soluble in alcohol and NH <sub>3</sub> .
AMTIR GeAsSe Glass	11,000-900 (0.9-11)	2.50	~ 18%	170	Insoluble in water. Soluble in bases.
Zinc Selenide ZnSe	20,000-500 (0.5-20)	2.43	~ 17%	150	Soluble in strong acids; dissolves in HNO <sub>3</sub> .
Silver Chloride AgCl	23,000-400 (0.42-25)	2.00	~ 11%	10	Insoluble in water; soluble in NH <sub>4</sub> OH.
Potassium Bromide KBr	33,000-400 (0.3-25)	1.54	~ 4.5 %	7	Soluble in water, alcohol, and glycerine; hygroscopic.
Cesium Iodide CsI	33,000-150 (0.3-70)	1.74	~ 7.3%	20	Soluble in water and alcohol; hygroscopic.
KRS-5 TlBr/l	16,000-200 (0.6-60)	2.38	~ 17%	40	Soluble in warm water; soluble in bases; insoluble in acids.
Polyethylene PE (high density)	600-10 (16-1,000)	1.52	~ 4.5%	5	Resistant to most solvents.
Diamond C	45,000-10 (0.22-1,000)	2.40	~ 17%	7000	Insoluble in water, acids, and bases.
TPX <sup>TM</sup> Methylpentene Resin	350-10 (28-1,000)	1.43	~ 3.3%		Similar to PE but transparent and more rigid







2400	2300	2200	2100	2000	1900 $\text{cm}^{-1}$	
				w		$-\text{C}\equiv\text{CH}$
			v			$-\text{C}\equiv\text{C}-$
			v			$-\text{C}\equiv\text{N}$
	s					$-\text{N}_2^+$
			s			$-\text{S}-\text{C}\equiv\text{N}$
s						$\text{CO}_2$
		s				$-\text{NCO}$
		s				$-\text{N}_3$
		s				$-\text{N}=\text{C}=\text{N}-$
		s				$>\text{C}=\text{C}=\text{O}$
		s				$-\text{N}=\text{C}=\text{S}$
		s				$>\text{C}=\text{N}=\text{N}$
			s			$>\text{C}=\text{C}=\text{N}-$
				s		$>\text{C}=\text{C}=\text{C}<$

**Positions of Stretching Vibrations of Triple Bonds and Cumulated Double Bonds**  
(s = strong, m = medium, w = weak, v = varying)

1800	1700	1600	1500	1400 $\text{cm}^{-1}$	
			m		$-\text{NH}_2$
				w	$>\text{NH}$
			s	s	$-\text{NH}_3^+$
		v			$>\text{C}=\text{N}-$
		v			$\begin{array}{c} \text{C}=\text{N} \\ \diagdown \\ \text{C}=\text{C} \end{array}$
				v	conj. cycl. $>\text{C}=\text{N}-$
			v		$-\text{N}=\text{N}-$
					$\begin{array}{c} \text{O}^- \\   \\ -\text{N}^+=\text{N}- \end{array}$
m-w					$>\text{C}=\text{C}<$
			m		$>\text{C}=\text{C}<$ Aryl conj.
	s		s		Dienes, Trienes etc.
			s		$\begin{array}{c} \text{CO}^- \\   \\ \text{C}=\text{C} \end{array}$
		s	one or two bands		$\begin{array}{c} \text{C}=\text{C} \\ \diagdown \quad \diagup \\ \text{N} \quad \text{O} \end{array}$
			m	m	Benzenes, Pyridines etc.
				s	$\text{C}-\text{NO}_2$
		s			$-\text{O}-\text{NO}_2$
			s		$>\text{N}-\text{NO}_2$
				s	$\text{C}-\text{N}=\text{O}$
	two bands		s		$-\text{O}-\text{N}=\text{O}$
				s	$>\text{N}-\text{N}=\text{O}$
				s	$-\text{CS}-\text{NH}-$

**Positions of the Double Bond Stretching Vibrations and N-H Bending Vibrations**  
(s = strong, m = medium, w = weak, v = varying)

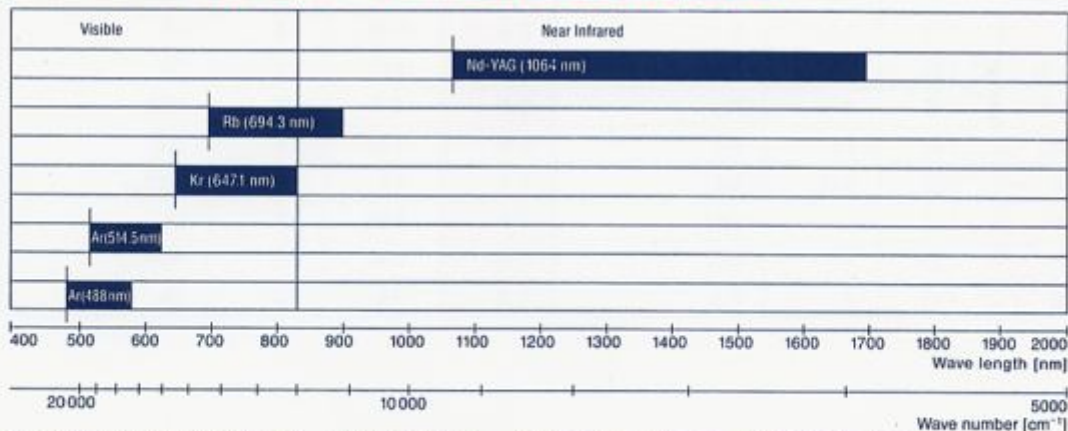
1900	1800	1700	1600	1500 $\text{cm}^{-1}$	
Dark	Dark	Dark			Aldehydes
Dark	Dark	Dark			Acid chlorides
Dark	Dark	Dark			Peracids
Dark	Dark	Dark			Saturated esters
Dark	Dark	Dark			Aryl- and $\alpha, \beta$ -unsaturated esters
Dark	Dark	Dark			-CO-O-C=C
Dark	Dark	Dark			$\alpha$ -Halogen esters and $\alpha$ -ketoesters
Dark	Dark	Dark			5-Ring lactones
Dark	Dark	Dark			$\alpha, \beta$ -Unsaturated 5-ring lactones
Dark	Dark	Dark			$\beta, \gamma$ -Unsaturated 5-ring lactones
Dark	Dark	Dark			4-Ring lactones
Dark	Dark	Dark			Aldehydes, ketones or esters with intramolecular H-bonds
Dark	Dark	Dark			Saturated aldehydes
Dark	Dark	Dark			Aryl- and unsaturated aldehydes
Dark	Dark	Dark			Saturated ketones
Dark	Dark	Dark			Aryl- and $\alpha, \beta$ -unsaturated ketones
Dark	Dark	Dark			$\alpha, \beta, \alpha', \beta'$ -Unsaturated ketones, quinones
Dark	Dark	Dark			5-Ring ketones
Dark	Dark	Dark			4-Ring ketones
Dark	Dark	Dark			$\alpha$ -Halogen- and $\alpha, \alpha'$ -dihalogen ketones
Dark	Dark	Dark			1, 2-Diketone
Dark	Dark	Dark			Saturated carboxylic acids
Dark	Dark	Dark			Aryl- and $\alpha, \beta$ -unsaturated carboxylic acids
Dark	Dark	Dark			$\alpha$ -Halogen carboxylic acids
Dark	Dark	Dark			Carboxylat ions
Dark	Dark	Dark			Primary amides in solution
Dark	Dark	Dark			Primary amides in solid state
Dark	Dark	Dark			<i>N</i> -methylsubst. amides in solution
Dark	Dark	Dark			<i>N</i> -monosubst. amides in solid state
Dark	Dark	Dark			<i>N, N</i> -disubst. amides
Dark	Dark	Dark			Lactams
Dark	Dark	Dark			Imides
Dark	Dark	Dark			Urethanes
Dark	Dark	Dark			R-CO-S-R'

Positions of Carbonyl Stretching Vibrations (all bands are strong)

1500	1400	1300	1200	1100	1000	900	800	700 $\text{cm}^{-1}$	
m		m						w	Alkanes
		s							-OCOCH <sub>3</sub> and -COCH <sub>3</sub>
m		s							-C(CH <sub>3</sub> ) <sub>3</sub>
s									>C(CH <sub>3</sub> ) <sub>2</sub> (Double band)
					s				-CH=CH- <i>trans</i>
					s/m				C=C-H Alkenes
		s							-O-H
		s							C-O
							s		5 neighbouring aromatic C-H
							s		4 neighbouring aromatic C-H
							s		3 neighbouring aromatic C-H
							s		2 neighbouring aromatic C-H
						w			1 isolated aromatic C-H
	s								C-NO <sub>2</sub>
			s						O-NO <sub>2</sub>
			s						N-NO <sub>2</sub>
s									N-N=O
			s					s	>N <sup>+</sup> -O <sup>-</sup>
					s				>C=S
s									-CSNH-
					s				>SO
					s				>SO <sub>2</sub>
		s							-SO <sub>2</sub> N<
		s							-SO <sub>2</sub> O-
	s								P-O-Alkyl
									P-O-Aryl
									>P=O
		s							>P(=O)OH
									C-F
					s			s	C-Cl

Characteristic Absorptions in the Fingerprint Region (s = strong, m = medium, w = weak)

## Stokes Shifts (0-3500 $\text{cm}^{-1}$ ) of Various Laser Sources



Nd-YAG: Neodymium YAG Laser

Rb: Ruby Laser

Kr: Krypton Ion Laser

Ar: Argon Ion Laser

## Selected Force Constants and Bond Orders (according to Siebert) of Organic and Inorganic Compounds

Bond A-B	Force Const. $f$ (N cm <sup>-1</sup> )	Bond Order	Compound	Bond A-B	Force Const. $f$ (N cm <sup>-1</sup> )	Bond Order	Compound
H-H	5.14	0.77	H <sub>2</sub>	H-O	7.40	1.0	HO <sup>-</sup>
Li-Li	1.24	1.2	Li <sub>2</sub>	H-F	8.85	1.1	HF
B-B	3.58	1.2	B <sub>2</sub>	H-Al	1.76	0.60	AlH <sub>4</sub> <sup>-</sup>
C-C	16.5	3.2	HCCH	H-Si	2.98	0.84	SiH <sub>4</sub>
N-N	22.42	3.2	N <sub>2</sub>	H-P	3.11	0.82	PH <sub>3</sub>
O-O	11.41	1.4	O <sub>2</sub>	H-S	4.29	1.0	H <sub>2</sub> S
F-F	4.45	0.58	F <sub>2</sub>	H-Cl	4.81	1.0	HCl
Na-Na	0.17	0.24	Na <sub>2</sub>	H-Ge	2.81	0.82	GeH <sub>4</sub>
Si-Si	4.65	2.0	Si <sub>2</sub>	H-As	2.85	0.81	AsH <sub>3</sub>
Si-Si	~1.7	~0.9	Si <sub>2</sub> H <sub>6</sub>	H-Se	3.51	0.93	H <sub>2</sub> Se
P-P	5.56	2.1	P <sub>2</sub>	H-Br	3.84	0.98	HBr
P-P	2.07	0.95	P <sub>4</sub>	H-Sn	2.03	0.76	SnH <sub>4</sub>
S-S	4.96	1.7	S <sub>2</sub>	H-Sb	2.09	0.77	SbH <sub>3</sub>
S-S	2.5	0.99	S <sub>8</sub>	H-I	2.92	0.97	HI
Cl-Cl	3.24	1.1	Cl <sub>2</sub>	C-H	5.50	1.0	CH <sub>4</sub>
Ni-Ni	0.11	0.2	Ni solid	C-B	3.82	1.1	B(CH <sub>3</sub> ) <sub>3</sub>
As-As	3.91	1.8	As <sub>2</sub>	C-C	16.5	3.2	HCCH
Se-Se	3.61	1.6	<sup>80</sup> Se <sub>2</sub>	C-C	9.15	1.9	H <sub>2</sub> CCH <sub>2</sub>
Br-Br	2.36	1.1	Br <sub>2</sub>	C-C	7.6	1.7	C <sub>6</sub> H <sub>6</sub>
Rb-Rb	0.08	0.2	Rb <sub>2</sub>	C-C	4.4	1.1	H <sub>3</sub> CCH <sub>3</sub>
Cd-Cd	1.11	1.0	Cd <sub>2</sub> <sup>2+</sup>	C-N	18.07	3.0	HCN
Sb-Sb	2.61	1.9	Sb <sub>2</sub>	C-N	11.84	2.1	CN <sub>2</sub> <sup>2-</sup>
Te-Te	2.37	1.7	Te <sub>2</sub>	C-N	6.54	1.3	NNCH <sub>2</sub>
I-I	1.70	1.2	I <sub>2</sub>	C-O	18.56	2.8	CO
Hg-Hg	1.69	1.5	Hg <sub>2</sub> <sup>2+</sup>	C-O	15.61	2.4	CO <sub>2</sub>
Pb-Pb	4.02	3	Pb <sub>2</sub>	C-O	12.76	2.0	OCH <sub>2</sub>
Bi-Bi	1.84	1.6	Bi <sub>2</sub>	C-O	7.86	1.3	CO <sub>3</sub> <sup>2-</sup>
H-B	2.75	0.68	BH <sub>3</sub>	C-O	5.1	0.96	O(CH <sub>3</sub> ) <sub>2</sub>
H-C	5.50	1.0	CH <sub>4</sub>	C-F	6.98	1.1	CF <sub>4</sub>
H-N	7.05	1.1	NH <sub>3</sub>	C-P	8.95	2.4	HCP
H-O	8.45	1.1	H <sub>2</sub> O	C-S	7.67	2.0	CS <sub>2</sub>

## Selected Force Constants and Bond Orders (according to Siebert) of Organic and Inorganic Compounds

Bond A-B	Force Const. f (N cm <sup>-1</sup> )	Bond Order	Compound	Bond A-B	Force Const. f (N cm <sup>-1</sup> )	Bond Order	Compound
C-S	3.3	1.0	S(CH <sub>3</sub> ) <sub>2</sub>	O-O	6.18	0.89	O <sub>2</sub> <sup>-</sup>
C-Cl	3.12	0.93	CCl <sub>4</sub>	O-O	5.70	0.83	O <sub>3</sub>
C-Ni	2.91	1.2	Ni <sub>4</sub> CO	O-Na	~3.2	~1.1	Na-OH
C-Ni	1.43	0.68	NiCO	O-Mg	3.5	1.1	MgO
C-Se	5.94	1.8	CSe <sub>2</sub>	O-Al	5.66	1.5	AlO
C-Br	2.42	0.86	CBr <sub>4</sub>	O-Al	3.8	1.1	Al(OH) <sub>4</sub> <sup>-</sup>
C-Rh	2.4	1.2	(Rh(CN) <sub>6</sub> ) <sup>3-</sup>	O-Si	9.25	2.1	SiO
C-Ag	2.0	0.99	(Ag(CN) <sub>2</sub> ) <sup>-</sup>	O-Si	4.75	1.2	SiO <sub>4</sub> <sup>4-</sup>
C-I	1.69	0.79	Cl <sub>4</sub>	O-P	9.41	2.0	PO
N-H	7.05	1.1	NH <sub>3</sub>	O-P	6.16	1.4	PO <sub>4</sub> <sup>3-</sup>
N-B	7.2	1.6	BN <sub>3</sub> <sup>3-</sup>	O-S	10.01	2.0	SO <sub>2</sub>
N-C	18.07	3.0	HCN	O-Cl	4.26	1.0	ClO <sub>2</sub> <sup>-</sup>
N-N	22.42	3.2	N <sub>2</sub>	O-Cl	3.30	0.82	ClO <sup>-</sup>
N-N	16.01	2.4	N-NNH	O-Ca	2.85	1.2	CaO
N-N	13.15	2.0	N-N-N <sup>-</sup>	O-Ti	7.19	2.4	TiO
N-O	25.07	3.1	N-O <sup>+</sup>	O-V	7.36	2.3	VO
N-O	17.17	2.3	NO <sub>2</sub> <sup>+</sup>	O-Cr	5.82	1.9	CrO
N-O	15.49	2.1	NO	O-Mn	5.16	1.6	MnO
N-O	15.18	2.0	ONCl	O-Fe	5.67	1.7	FeO
N-O	11.78	1.7	NNO	O-Cu	2.97	0.93	CuO
N-F	4.16	0.66	NF <sub>3</sub>	O-Ge	7.53	1.8	<sup>74</sup> GeO
N-Si	3.8	1.1	((CH <sub>3</sub> ) <sub>3</sub> Si) <sub>2</sub> NH	O-Se	6.45	1.5	SeO
N-S	12.54	2.5	NSF <sub>3</sub>	O-Mo	3.05	1.2	Ba <sub>2</sub> CaMoO <sub>6</sub> (solid)
N-S	8.3	1.9	HNSO	O-Ru	6.70	2.2	RuO <sub>4</sub>
N-S	3.1	0.87	H <sub>3</sub> N-SO <sub>3</sub>	O-Ag	2.00	0.79	AgO
O-Li	1.58	0.66	LiO	O-Sn	5.53	1.7	SnO
O-Be	7.51	1.8	BeO	O-Te	5.31	1.6	TeO
O-B	13.66	2.5	BO	O-Ba	3.79	1.8	BaO
O-B	6.35	1.3	BO <sub>3</sub> <sup>3-</sup>	O-Ce	6.33	2.6	CeO
O-O	16.59	2.0	O <sub>2</sub> <sup>+</sup>	O-Pr	5.68	2.4	PrO
O-O	11.41	1.4	O <sub>2</sub>	O-Nd	3.5	1.6	NdAc <sub>3</sub> ·H <sub>2</sub> O (polymer)

## Properties of Some Important Solvents

Solvent	Abbreviation	Formula	Molecular weight	F. p. (°C)	B. p. (°C)	Density	Dipole Mom.*	Susceptib. $\chi \cdot 10^6$	Di-electr. Const.	Refract. Index	Chemical Shift	
											$\delta$ <sup>1</sup> H (ppm)	$\delta$ <sup>13</sup> C (ppm)
Acetic acid		C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	60.0 <sub>5</sub>	16.7	117.9	1.049	1.2	0.551(32°)	6.1	1.3719	2.1	21.1 177.3
Acetone	AC	C <sub>3</sub> H <sub>6</sub> O	58.1	-94.7	56.3	0.790	2.88	0.460	20.7	1.3587	2.05	30.50 205.1
Acetonitrile	AN	C <sub>2</sub> H <sub>3</sub> N	41.0 <sub>5</sub>	-44	81.6	0.777	3.92	0.534	37.5	1.3416	1.93	1.28 118.10
Benzene*		C <sub>6</sub> H <sub>6</sub>	78.1	5.5	80.1	0.879	0	0.699 (22°)	2.3	1.5011	7.16	128.70
t-Butyl alcohol	t-BuOH	C <sub>4</sub> H <sub>10</sub> O	74.1	25.5	82.2	0.789	1.66	0.534	1.8	1.3878	1.3	31.6 68.7
Carbon disulfide		CS <sub>2</sub>	76.1	-111.6	46.2	1.270	0	0.532	2.6	1.6319		192.8
Carbon tetrachloride*		CCl <sub>4</sub>	153.8	-23	76.7	1.584	0	0.691	2.2	1.4574		96.7
Chloroform*		CHCl <sub>3</sub>	119.4	-63.5	61.1	1.480	1.01	0.740	4.8	1.4429	7.26	77.36
Cyclohexane		C <sub>6</sub> H <sub>12</sub>	84.2	6.6	80.7	0.774	0	0.627	2.0	1.4235	1.4	27.8
Cyclopentane		C <sub>5</sub> H <sub>10</sub>	70.1	-93.8	49.3	0.745		0.629	2.0	1.4065	1.5	26.5
Decaline		C <sub>10</sub> H <sub>18</sub>	138.2	-43	191.7	0.879		0.681		1.4758	0.9 to 1.8	24 to 44
Dibromomethane		CH <sub>2</sub> Br <sub>2</sub>	173.8	-52.6	97.0	1.5420	1.43	0.935	7.5	2.497	5.0	21.6
o-Dichlorobenzene*	ODCB	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	147.0	-17	180.5	1.306	2.50	0.748	9.9	1.5515	7.0 to 7.4	128 to 133
Diethylether		C <sub>4</sub> H <sub>10</sub> O	74.1	-116.2	34.5	0.7138	1.15		4.3	1.3526	1.2 3.5	17.1 67.4
1,2-Dichloroethane		C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	99.0	-35.7	83.5	1.246	1.75		10.4	1.4421	3.7	51.7
1,2-Dichloroethylene Z		C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	96.9	-80.0	60.6	1.284	1.90	0.679 (15°)	9.2	1.4490	6.4	119.3
1,2-Dichloroethylene E		C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	96.9	-49.8	47.7	1.255	0	0.638 (15°)	2.1	1.4462	6.3	121.1
1,1-Dichloroethylene		C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	96.9	-122.6	31.6	1.213	1.34	0.635 (15°)	4.6	1.4247	5.5	115.5 128.9
Dichloromethane		CH <sub>2</sub> Cl <sub>2</sub>	84.9	-95.1	39.8	1.315	1.60	0.733	8.9	1.4211	5.31	53.73
Dimethoxymethane		C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	76.1	-105.2	42.3	0.866		0.611	2.6	1.3563	3.3 4.4	54.8 97.9
Dimethylacetamide	DMA	C <sub>4</sub> H <sub>9</sub> NO	87.1	-20.0	166.1	0.937	3.8		37.8	1.4356	2.1 3	34/38 169.6
Dimethylcarbonate*		C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	90.1	3	90.5	1.069				1.3687	3.65	54.8 156.9
Dimethylether		C <sub>2</sub> H <sub>6</sub> O	46.1	-139	-24							59.4
N,N-Dimethylformamide	DMF	C <sub>3</sub> H <sub>7</sub> NO	73.1	-60.4	153.0	0.944	3.86		36.7	1.4282	2.9 8.0	30.10 35.2 162.5
Dimethylsulfoxide	DMSO	C <sub>2</sub> H <sub>6</sub> SO	78.1	18.5	189.0	1.096	3.96		46.7	1.4773	2.49	39.50
Dioxane*	D	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	88.1	11.8	101.3	1.028	0.45	0.606 (32°)	2.2	1.4203	3.53	66.30



## Properties of Some Important Solvents

Solvent	Abbreviation	Formula	Molecular weight	F. p. (°C)	B. p. (°C)	Density	Dipole Mom.**	Susceptib. $\chi \cdot 10^6$	Dielectr. Const.	Refract. Index	Chemical Shift	
											$\delta$ <sup>1</sup> H (ppm)	$\delta$ <sup>13</sup> C (ppm)
Ethanol	EtOH	C <sub>2</sub> H <sub>5</sub> O	46.1	-114.1	78.3	0.785	1.69	0.575	24.5	1.3594	1.10	17.20 56.70
Ethyl acetate		C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	88.1	-83.9	77.1	0.895	1.8	0.554	6.0	1.3698	1.2/2.0 4.1	14.3 60.1 170.4
Ethylene carbonate	EC	C <sub>3</sub> H <sub>2</sub> O <sub>3</sub>	88.1	36.4	238	1.321	4.91		89.6	1.4250	4.4	65.0 155.8
Freon 12		CF <sub>2</sub> Cl <sub>2</sub>	120.9	-158	-29.8	1.18	0.5	0.642 (30°)				
Freon 22		CHClF <sub>2</sub>	86.5	-146	-40.8	1.491	1.4					
Formamide	F	CH <sub>3</sub> ON	45.0	2.6	210.5	1.133	3.73	0.551	109	1.4475	7.2 8.1	165.1
Hexachloroacetone		C <sub>3</sub> Cl <sub>6</sub> O	264.8	-30	203	1.744				1.5112		123.7 126.4
Hexafluorodichloropropane		C <sub>3</sub> F <sub>4</sub> Cl <sub>2</sub>	220.9	-136	35	1.589						
Hexamethylphosphoramide*	HMPT	C <sub>6</sub> H <sub>18</sub> N <sub>3</sub> PO	179.2	7.2	233	1.027	5.39		30.0	1.4588	2.4 2.6	36.6
Methanol	MeOH	CH <sub>3</sub> O	32.0	-97.7	64.7	0.787	1.70	0.530	32.7	1.3265	3.31	49.0
Methyl chloride		CH <sub>3</sub> Cl	50.5	-97.7	-24.1	0.916	1.87		12.6	1.3389		25.1
Morpholine		C <sub>4</sub> H <sub>9</sub> NO	87.1	-3.1	128.9	1.005		0.631	7.4	1.4573	2.6 3.9	46.8 68.9
Nitromethane		CH <sub>3</sub> NO <sub>2</sub>	61.0	-28.5	101.2	1.131	3.46	0.391 (25°)	35.9	1.3796	4.33	62.80
Pyridine		C <sub>5</sub> H <sub>5</sub> N	79.1	-41.6	115.3	0.978	2.2	0.611	12.4	1.5075	7.21 7.57 8.72	123.50 135.50 149.50
Quinoline		C <sub>8</sub> H <sub>7</sub> N	129.2	-14.9	237.1	1.098	2.2	0.729	9.0	1.6293	7 to 8.8	121 to 151
Sulfur dioxide		SO <sub>2</sub>	64.1	-72.7	-10.0	1.434	1.6		17.6			
2,2-Tetrachloroethane		C <sub>2</sub> H <sub>2</sub> Cl <sub>4</sub>	167.8	-43.8	146.2	1.578	1.3	0.856	8.2	1.4868	6.0	74.0
Tetrachloroethane		C <sub>2</sub> Cl <sub>4</sub>	165.8	-22.3	121.2	1.631		0.802 (15°)	2.3	1.5076		120.4
Tetrahydrofuran	THF	C <sub>4</sub> H <sub>8</sub> O	72.1	-66	66.0	0.889	1.75		7.6	1.4050	1.72 3.57	25.26 67.2
Tetramethylurea	TMU	C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> O	116.2	-1.2	176.5	0.969	3.47	0.634 (15°)	23.1	1.4459	2.8	38.5 165.6
Toluene		C <sub>7</sub> H <sub>8</sub>	92.1	-94.9	110.6	0.867	0.36	0.618	2.4	1.4969	2.09 7.01 7.09	21.3 138.5
Trichloroethylene*		C <sub>2</sub> CHCl <sub>3</sub>	131.4	-73	87.2	1.476		0.734	3.4	1.4800	6.4	116.7 124.0
Water		H <sub>2</sub> O	18.02	0	100	0.997	1.85	0.719	78.5	1.3329	4.72	

B.p.: boiling point      F.p.: freezing point      Reference of the shifts: <sup>1</sup>H and <sup>13</sup>C (TMS)

\*\* Dipole moment in Debye units: (1D = 10<sup>-18</sup> e.s.u. cm  $\approx$  3.3356 x 10<sup>-30</sup> C m)

\* Carcinogens or cancer suspect agents

## SI Unit System (Système International)

Fundamental SI Quantities	Name	Symbol	
Length	Meter	m	
Mass	Kilogram	kg	
Time	Second	s	
Electric Current	Ampere	A	
Thermodynamic Temperature	Kelvin	K	
Amount of Substance	Mole	mol	
Light Intensity, Luminosity	Candela	cd	
Special SI-derived Quantities	Name	Symbol	Units
Frequency	Hertz	Hz	$s^{-1}$
Plane Angle			$2\pi \text{ rad} = 360^\circ$ , $1 \text{ rad} = 57.2957795^\circ$
Angular Frequency	Radian	rad	$\text{rad s}^{-1}$ [ $1 \text{ Hz} = 2\pi \text{ rad s}^{-1}$ ]
Solid Angle	Steradian	sr	$4\pi \text{ sr} = \text{sphere}$
Force	Newton	N	$\text{m kg s}^{-2}$
Pressure, Stress	Pascal	Pa	$\text{N m}^{-2} = \text{m}^{-1} \text{ kg s}^{-2}$ [ $1 \text{ bar} = 10^5 \text{ Pa}$ ]
Energy, Work, Heat	Joule	J	$\text{N m} = \text{m}^2 \text{ kg s}^{-2}$
Power, radiant flux	Watt	W	$\text{J s}^{-1} = \text{m}^2 \text{ kg s}^{-3}$
Electric Charge	Coulomb	C	$\text{A s}$
Electric potential, emf	Volt	V	$\text{J C}^{-1} = \text{m}^2 \text{ kg s}^{-3} \text{ A}^{-1}$
Electrical Resistance	Ohm	$\Omega$	$\text{V A}^{-1} = \text{m}^2 \text{ kg s}^{-3} \text{ A}^{-2}$
Electrical Conductance	Siemens	S	$\Omega^{-1} = \text{m}^{-2} \text{ kg}^{-1} \text{ s}^3 \text{ A}^2$
Electrical Capacitance	Farad	F	$\text{C V}^{-1} = \text{m}^{-2} \text{ kg}^{-1} \text{ s}^4 \text{ A}^2$
Magnetic Flux	Weber	Wb	$\text{V s} = \text{m}^2 \text{ kg s}^{-2} \text{ A}^{-1}$
Magnetic Flux Density	Tesla	T	$\text{Wb m}^{-2} = \text{V s m}^{-2} = \text{kg s}^{-2} \text{ A}^{-1}$
Inductance	Henry	H	$\text{V A}^{-1} \text{ s} = \text{m}^2 \text{ kg s}^{-2} \text{ A}^{-2}$
Celsius Temperature	$^\circ\text{C}$	K	$^\circ\text{C} = \text{Temp.}(\text{K}) - 273.15$
Light Flux	Lumen	lm	$\text{cd sr}$
Illuminance	Lux	lx	$\text{cd sr m}^{-2}$
Activity (radioactive decay)	Becquerel	Bq	$s^{-1}$ [ $1 \text{ Curie (Ci)} = 37 \text{ GBq}$ ]
Absorbed Dose	Gray	Gy	$\text{J kg}^{-1} = \text{m}^2 \text{ s}^{-2}$ [ $1 \text{ rad} = 0.01 \text{ Gy}$ ]
Equivalent Dose, Energy Dose	Sievert	Sv	$\text{J kg}^{-1} = \text{m}^2 \text{ s}^{-2}$ [ $1 \text{ rem} = 0.01 \text{ Sv}$ ]
Other Quantities	Name	Symbol	Units
Volume	Liter	L or l	$\text{dm}^3 = 10^{-3} \text{ m}^3 = 10^3 \text{ cm}^3$
Length	Ångström	Å	$10^{-10} \text{ m}$
Energy	Electron Volt	eV	$1.6021764 \times 10^{-19} \text{ J}$
Viscosity		$\eta$	$\text{Pa s}$
Diffusion Constant		$D$	$\text{m}^2 \text{ s}^{-1}$
Molar Energy			$\text{J mol}^{-1} = \text{m}^2 \text{ kg s}^{-2} \text{ mol}^{-1}$
Molar Entropy			$\text{J K}^{-1} \text{ mol}^{-1} = \text{m}^2 \text{ kg s}^{-2} \text{ K}^{-1} \text{ mol}^{-1}$
Electric Field Strength		$E$	$\text{V m}^{-1} = \text{m kg s}^{-3} \text{ A}^{-1}$
Magnetic Field Strength		$H$	$\text{A m}^{-1} = \text{N m}^{-2} \text{ T}^{-1} = \text{Pa T}^{-1}$

# Conversion Factors for Important Physical Units

## Energy Equivalents

	Joule	Hertz	cm <sup>-1</sup>	Kelvin	eV
Joule	1	1.5091905 E+33	5.03411762 E+22	7.242964 E+22	6.24150974 E+18
Hertz	6.62606876 E-34	1	3.335640952 E-11	4.7992374 E-11	4.13566727 E-15
cm <sup>-1</sup>	1.98644544 E-23	2.99792458 E+10	1	1.4387752	1.239841857 E-04
Kelvin	1.3806503 E-23	2.0836644 E+10	0.6950356	1	8.617342 E-05
eV	1.602176462 E-19	2.417989491 E+14	8.06554477 E+03	1.1604506 E+04	1

(based on the Fundamental Constants with  $E = mc^2 = hc/\lambda = h\nu = kT$  and  $1 \text{ eV} = (e/C) \text{ J}$ )

## Force Units (SI unit = Newton, cgs unit = dyne), Weight = mass $\times$ $g_n$

	N	p (pond)	kp	dyne
N	1	101.9716	0.1019716	1.0 E+05
p	0.00980665	1	1.00 E-03	980.665
kp	9.80665	1000	1	980665
dyne	1.0 E-05	1.019716 E-03	1.019716 E-06	1

## Energy and Work Units (SI unit = Joule, cgs unit: 1 erg = 10<sup>-7</sup> Joule)

	J = N m	kp m	kWh	kcal	BTU	eV
J	1	0.101972	2.777778 E-07	2.390057 E-04	9.478134 E-04	6.241512 E+18
kp m	9.80665	1	2.724069 E-06	2.343846 E-03	9.294874 E-03	6.120832 E+19
kWh	3.600 E+06	3.670978 E+05	1	860.4207	3412.128	2.246944 E+25
kcal	4184	426.6493	1.162222 E-03	1	3.965651	2.611448 E+22
BTU	1055.06	1.075862 E+02	2.930722 E-04	2.521654 E-01	1	6.585169 E+21
eV	1.602176 E-19	1.633765 E-20	4.450489 E-26	3.829293 E-23	1.518564 E-22	1

## Power Units (SI unit = Watt)

	W = J s <sup>-1</sup>	kW	kpm/s	PS	cal/s	kcal/h
W	1	1.0 E-03	0.1019716	1.341022 E-03	0.2390057	0.8604207
kW	1.0 E+03	1	101.9716	1.341022	239.0057	860.4207
kpm/s	9.80665	9.80665 E-03	1	1.315093 E-02	2.343846	8.437844
PS	745.7	0.7457	76.04024	1	178.2266	641.8157
cal/s	4.184	4.184 E-03	0.4266493	5.610835 E-03	1	3.6
kcal/h	1.162222	1.162222 E-03	0.1185137	1.558565 E-03	0.2777778	1

## Pressure Units (SI unit = Pascal)

	Pa=N/m <sup>2</sup>	kp/m <sup>2</sup>	atm	bar	Torr=mmHg	at=kp/cm <sup>2</sup>
Pa=N/m <sup>2</sup>	1	0.1019716	9.86923 E-06	1.0 E-05	7.500617 E-03	1.019716 E-05
kp/m <sup>2</sup>	9.80665	1	9.67841 E-05	9.80665 E-05	7.355592 E-02	1.0 E-04
atm	1.01325 E+05	1.033227 E+04	1	1.01325	760	1.033227
bar	1.0 E+05	1.019716 E+04	0.9869233	1	750.0617	1.019716
Torr	133.3224	13.59510	1.315789 E-03	1.333224 E-03	1	1.359510 E-03
at=kp/cm <sup>2</sup>	9.80665 E+04	1.0 E+04	0.9678411	9.80665 E-01	735.5592	1

## Time Units (SI unit = second)

	s	min	h	d	week	year
s	1	1.666667 E-02	2.777778 E-04	1.157407 E-05	1.653439 E-06	3.168874 E-08
min	60	1	1.666667 E-02	6.944444 E-04	9.920635 E-05	1.901324 E-06
h	3600	60	1	4.166667 E-02	5.952381 E-03	1.140795 E-04
d	86400	1440	24	1	1.428571 E-01	2.737907 E-03
week	604800	10080	168	7	1	1.916535 E-02
year	31556952	525949.2	8765.82	365.2425	52.1775	1

## Temperature Conversion (SI unit = Kelvin)

	Kelvin (K)	Centigrade (°C)	Fahrenheit (°F)	Rankine (°R)
K	1	$T_C = T_K - 273.15$	$T_F = (9/5)T_K - 459.67$	$T_R = (9/5)T_K$
°C	$T_K = T_C + 273.15$	1	$T_F = (9/5)T_C + 32$	$T_R = (9/5)(T_C + 273.15)$
°F	$T_K = (5/9)(T_F + 459.67)$	$T_C = (5/9)(T_F - 32)$	1	$T_R = T_F + 459.67$
°R	$T_K = (5/9)T_R$	$T_C = (5/9)T_R - 273.15$	$T_F = T_R - 459.67$	1

## Tubing Diameters and Volumes

Inches (")	No. of Wire Gage*	Millimeters (mm)	Microns (µm)	Volume µl/in	Volume µl/cm
0.001	49	0.025	25	0.013	0.005
0.002	44	0.051	51	0.051	0.020
0.003	40	0.076	76	0.114	0.045
0.004	37	0.102	102	0.206	0.081
0.005	36	0.127	127	0.323	0.127
0.006	34	0.152	152	0.460	0.181
0.007	33	0.178	178	0.632	0.249
0.008	32	0.203	203	0.820	0.323
0.009	31	0.229	229	1.046	0.412
0.010	30	0.254	254	1.288	0.507
0.011	29	0.279	279	1.552	0.611
0.012	28	0.305	305	1.854	0.730
0.013	-	0.330	330	2.172	0.855
0.014	27	0.357	357	2.540	1.000
0.015	26	0.381	381	2.896	1.140
0.016	-	0.406	406	3.287	1.294
0.017	-	0.432	432	3.721	1.465
0.018	25	0.457	457	4.163	1.639
0.019	-	0.483	483	4.650	1.831
0.020	24	0.508	508	5.146	2.026
0.030	21	0.762	762	11.577	4.558
0.040	18	1.016	1016	20.581	8.103
0.050	16	1.270	1270	32.160	12.660

\* Gages taken from the American Wire or Brown & Sharpe Gage.

## Metric to U. S. Conversion

Metric	Inches (")	U. S. (")	U. S. (")	Metric
1.00 mm	0.039	0.062	1/16	1.59 mm
1.80 mm	0.070	0.125	1/8	3.18 mm
2.00 mm	0.079	0.188	3/16	4.76 mm
3.00 mm	0.118	0.250	1/4	6.35 mm
3.20 mm	0.126	0.313	5/16	7.94 mm
4.00 mm	0.158	0.375	3/8	9.53 mm
4.30 mm	0.170	0.438	7/16	11.11 mm
4.60 mm	0.181	0.500	1/2	12.70 mm
5.00 mm	0.197	0.563	9/16	14.29 mm
6.00 mm	0.236	0.625	5/8	15.86 mm
7.00 mm	0.276	0.688	11/16	17.46 mm
8.00 mm	0.315	0.750	3/4	19.05 mm
9.00 mm	0.355	0.813	13/16	20.64 mm
1.00 cm	0.394	0.875	7/8	22.22 mm
2.00 cm	0.788	0.938	15/16	23.81 mm
3.00 cm	1.182	1.00	1	2.54 cm
4.00 cm	1.576	2.00	2	5.08 cm
5.00 cm	1.970	3.00	3	7.62 cm
6.00 cm	2.364	4.00	4	10.16 cm
7.00 cm	2.758	5.00	5	12.70 cm
8.00 cm	3.152	6.00	6	15.24 cm
9.00 cm	3.546	7.00	7	17.78 cm
10.00 cm	3.940	10.0	10	25.40 cm

## U. S. to Metric Conversion

## Temperature Conversions

Kelvin	Celcius	Fahrenheit
0	-273.15	-459.67
4.2	-268.95	-452.11
10	-263.15	-441.67
20	-253.15	-423.67
30	-243.15	-405.67
40	-233.15	-387.67
50	-223.15	-369.67
60	-213.15	-351.67
70	-203.15	-333.67
77.35	-195.8	-320.44
80	-193.15	-315.67
90	-183.15	-297.67
100	-173.15	-279.67
110	-163.15	-261.67
120	-153.15	-243.67
130	-143.15	-225.67
140	-133.15	-207.67
150	-123.15	-189.67
160	-113.15	-171.67
170	-103.15	-153.67
180	-93.15	-135.67
190	-83.15	-117.67
200	-73.15	-99.67
210	-63.15	-81.67
220	-53.15	-63.67
230	-43.15	-45.67
240	-33.15	-27.67
250	-23.15	-9.67
255.37	-17.78	0
260	-13.15	8.33
270	-3.15	26.33
273.15	0	32
280	6.85	44.33
290	16.85	62.33
300	26.85	80.33
310	36.85	98.33
320	46.85	116.33
330	56.85	134.33
340	66.85	152.33
350	76.85	170.33
360	86.85	188.33
370	96.85	206.33
380	106.85	224.33
390	116.85	242.33
400	126.85	260.33
410	136.85	278.33
420	146.85	296.33
475	201.85	395.33

## Pressure Conversion

PSI	TORR	ATM	BAR
100	5170	6.8	6.7
500	25850	34.0	33.6
1000	51700	68.0	67.2
1500	77550	102.1	100.7
2000	103400	136.1	134.3
2500	129250	170.0	168.0
3000	155100	204.1	201.5
3500	180950	238.0	235.2
4000	206800	272.1	268.6
4500	232650	306.0	302.4
5000	258500	340.2	335.8
5500	284350	374.0	369.6
6000	310200	408.2	402.9
6500	336050	442.0	436.8
7000	361900	476.3	470.1
7500	387750	510.0	504.0
8000	413600	544.0	537.6
8500	439450	578.0	571.2
9000	465300	612.0	604.8
10000	517000	680.4	671.5

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