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Mobilities In Organic Molecular Crystals

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Mobilities In Organic Molecular Crystals

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A complete list of mobilities in molecular organic crystals is presented. This updates the 1977 list and includes many new developments in the field.

Charge transport properties of molecular crystals are of interest because the magnitude and temperature dependences of the mobilities μ exhibit a remarkable trend independent of the particular material and such data challenges both band and hopping theories of charge transport. It is the purpose of this paper to present a complete list of mobility measurements in molecular crystals. Such a list will be useful as a guide to experimentalist who are considering expanding the list of characterized materials and theorists who are considering resolving the band, hopping issue associated with these materials. Such a list highlights the trend that, independent of the particular material,

$$\mu = 1 \text{ cm}^2/\text{Vsec}$$

within an order of magnitude at room temperature, and μ is almost always weakly temperature dependent

$$\mu \propto T^{-n} \text{ with } n = 1^{+2}_{-1}$$

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Lists of mobilities of molecular crystals can be found in some of the reviews[141-155] on the subjects; the last complete list was published in 1977.[122] Since then, many new developments have occured which should be documented including (1) the first[7,10] measurements below 77 K which revealed a sharp change in the temperature dependence of μ at 100 K for electrons in the c' direction of naphthalene, (2) observations of high mobilities at low temperatures (order of magnitude 100 $cm^2/Vsec$) in durene[58-60] and perylene,[78] (3) the first measurements of the off-diagonal components of the mobility tensor,[14,45,47] (4) measurements of many new materials including charge transfer complexes and (5) tests of the electric field[9,40,48] dependence of μ which has emerged as a crucial test of proposed transport theories.

A complete list (to the authors' knowledge) of mobilities, their magnitude, temperature and electric field dependence, is given in Table I. Such data, especially the temperature and electric field dependence μ, are critical tests of transport theories; the reader is referred to the literature for a more complete discussion of the issues. Only measurements of intrinsic mobilities (not impurity dominated mobilities) made by time of flight techniques are included in this table. The table lists the material, the sign of the carrier (+ represents holes, − represents electrons), the orientation in the crystal during the measurement, the room temperature value of the mobility and its error (where known), the temperature dependence and temperature range over which the temperature dependence was determined, and finally the electric field range over which the mobility for the various orientations was tested to be electric field independent (the one observation of a field dependent mobility is Ref. 48). Where more than one paper is referenced for a particular material, the most reliable values (in our judgement) are shown in Table I.

Excluded from this table are those measurements of the drift mobility which the data suggests were determined by impurities (n-terphenyl[130,131] and rubrene,[128] stilbene,[129] m-terphenyl,[129] ferrocene,[132] triphenylamine,[132] trans-stilbene[132] violanthrene,[133] phenanthrene-PMDA,[104-106] anthracene 1,3,5 trinitrobenzene[107,108] and phthalocyanine crystals[134-140]). Rare-gas solids,[126,127] which are not molecular, are also excluded. Also excluded are inorganic molecular crystals which generally exhibit the same trend (Se_8,[114,115] S_8,[116,117] As_4S_4,[118] I,[119,120] F,[121] As_2S_3,[122] S_4I_4[123]; for exceptions, see S_8,[116,117] and other layered semiconductors.[124]

TABLE 1

	Sign of carrier	Orientation	Room temp. mobility ($cm^2/Vsec$)	$\mu \propto T^n$ n	Temp. range (K)	E field range ($V/\mu m$)	References
Benzene	−	*a*	1.5(@ 278 K)	−2.0	173–278		1
Naphthalene	+	*a*	0.90 ± 0.01	−2.9 ± 0.1	78–300	2.9–17.3	2–15
	+	*b*	1.5 ± 0.1	−2.5 ± 0.3	78–300		15
	+	*c'*	0.30 ± 0.03	−2.82 ± 0.02	78–300		15
	+	*ac'*	−0.049 ± 0.005		300		14
	−	*a*	0.65 ± 0.1	−1.52 ± 0.05	78–300		15
	−	*b*	0.63 ± 0.05	exp(9 ± 1 meV/kT)	75–100		10
				?	100–300		
	−	*c'*	0.44 ± 0.01	exp(6.6 ± 0.1 meV/kT)	31–100		7, 10, 45, 47
				0.1 ± 0.1	100–325		
	−	*ac'*	−0.16 ± 0.03		300		14
Perdeuterated Naphthalene	+	*a*	0.78 ± 0.05	−2.8 ± 0.1	78–300	5.0–16.5	16–21
	+	*b*	1.6 ± 0.1	−2.5 ± 0.3	78–300		21
	+	*c'*	0.3 ± 0.1	−2.72 ± 0.04	78–300		21
	−	*a*	0.7 ± 0.1	−1.37 ± 0.03	78–300		18, 21
	−	*b*	0.53 ± 0.04	exp(8.4 ± 0.2 meV/kT)	78–100		17, 21
				?	100–300		
	−	*c'*	0.40 ± 0.01	exp(7.0 ± 1.0 meV/kT)	68–100		17, 21
				0.1 ± 0.1	100–323		
Anthracene	+	*a*	1.13 ± 0.02	−1.5 ± 0.2	78–300		22–53
	+	*b*	2.07 ± 0.04	−1.5 ± 0.2	78–300		45, 47
	+	*c'*	0.73 ± 0.02	−1.5 ± 0.2	78–300		45, 47
	+	*ac'*	−0.28 ± 0.01		100		45, 47

TABLE I (*continued*)

	Sign of carrier	Orientation	Room temp. mobility ($cm^2/Vsec$)	$\mu \propto T^n$ n	Temp. range (K)	E field range (V/μm)	References
			-1.8 ± 0.1		300		
	−	*a*	1.73 ± 0.03	−1.57	78–300		45, 47
	−	*b*	1.05 ± 0.02	−0.84	78–300		45, 47
	−	*c′*	0.39 ± 0.01	-0.16 ± 0.02	78–300		45, 47
	−	*ac′*	-0.05 ± 0.03		300		45, 47
			$+0.32 \pm 0.02$		150		
Perdeuterated Anthracene	+	*a*	1.1	-1.5 ± 0.1	150–325		45, 47, 54–56
	+	*b*	2.1	-1.40 ± 0.05	150–300		
	+	*c′*	0.73	−1.48	150–300		
	−	*a*	1.73	-1.5 ± 0.1	160–325		
	−	*b*	1.05	0.88	180–300		
	−	*c′*	0.35 ± 0.01	-0.10 ± 0.03	130–377		55
Durene	+	in *ab* plane	5.0(50 @ 120 K)	−2.5	130–300	57–60	
	+	*c′*	0.1	−2.8	130–300		
	−	in *ab* plane	8.0(30 @ 120 K)	−2.5	130–300		
Biphenyl	−	*a*	0.42	−1.0	135–300	1.8–4.2	61, 62
	−	*b*	1.25	−1.25	76–300		
	−	*c′*	0.51	−1.0	100–250		
Pyrene	+	in *ab* plane	0.7	−1.6	260–350		63–65
	+	*c′*	0.5	−1.3	260–350		
	−	in *ab* plane	0.7	−1.5	260–350		
	−	*c′*	0.5	−2.0	260–350		
Tetracene	+	*c′*	0.85 ± 0.05	$2 < n < 3$	300–350	0.1–10.0	66–70
TCNQ	−	⊥(001)	0.65 ± 0.1	−1.0	210–350	3–10	71, 72
Phenanthrene	+	*a*	0.68 ± 0.08				73
	+	*b*	1.1 ± 0.1				
	+	*c′*	0.12 ± 0.01				

1,4 Dibromonaphthalene	+	*a*	0.66	−2.0	270–300		74–76
	+	*b*	0.25	−2.0	270–300		
	+	*c′*	0.87	−2.0	270–300		
	−	*a*	0.017	−2.0	270–300		
	−	*b*	0.013	−2.0	270–300		
	−	*c′*	0.034	−2.0	270–300		
Perylene	−	non-principle	2(100 @ 30 K)	−1.7	30–300		77, 78
N-isopropyl carbazole	+	*c*	0.33			0.5–4	79, 80
	−	*c*	1.0	0	244–370		
p-diidobenzene	+	*a*	12.0	−0.5	250–300		81
				0	310–350		
	+	*b*	4.0	0	250–350		
	+	*c*	1.7	−0.8	250–320		
Phenazine	−	*a*	0.29	0	180–360		82
	−	*b*	1.1	−0.65	230–360		
	−	*c′*	0.5	−0.1	230–360		
Azulene	−	⊥(110)	0.2				83–85
	+	*c′*	0.19			~2.8	
Auramine	+		1.06(77 K)		77		86
Phenothiazine	−	⊥ to plane	5.0	−3.0	300–400		87
	−	in clev. plane	1.7	−3.0	300–350		
Anthraquinone	−	*a*	0.02				88, 89
	−	*b*	0.20				
	−	*c′*	0.28				
Benzophenone	−	*a*	0.16	0	230–300	1.1–4.0	90
	−	*c*	0.055	0	230–300		
β-9,10-dichloro-anthracene	+	in *ac* plane	0.6			0.7–2.6	91
	+	*b′*	0.18			0.7–2.6	
α-9,10-dichloro-anthracene	+	*a, b, c′*	3.8 ± 0.2	−2.4	183–295		92, 93
Tetracyanoethylene (TCNE)	+	1	0.21		245–355		94, 95
	+	2, *b*	0.10		245–355		

TABLE I (*continued*)

	Sign of carrier	Orientation	Room temp. mobility ($cm^2/Vsec$)	$\mu \propto T^n$ n	Temp. range (K)	E field range ($V/\mu m$)	References
	+	3	0.15		245–355		
Iodoform	+	‖-6 fold axis	0.18 ± 0.05	$0.2 < n < 1$	270–340		96
	+	⊥6 fold axis	0.7 ± 0.15		270–340		
p-terphenyl	−	*a*	0.34	−2.5	70–180	0.23–4.7	97, 98
				−0.5	180–300		
	−	*b*	1.2	−2.5	90–180		
				−0.7	180–300		
	−	*c'*	0.25		160–300		
	+	*c'*	0.8		160–300		
o-terphenyl	−	*b*	3	exp(−140 meV/kT)	210–270		99

				0	100–210		
dibenzothiophene	+	*a*	1.39				
	+	*b*	1.10				
	+	*c'*	1.6 ± 0.1	−2	295–360	0.33	100, 101
anthracene pyromellitic dianhydride	−	∥(010)	0.15 ± 0.01 (@ 353)	0	353–453	0	102, 103
	−	⊥(010)	0.02(@ 393)	−2.0	373–453		
n-isopropyl carbazole picryl chloride	+	*c*	0.33	exp(100 meV/kT)		.5–4	109, 110
	−	*c*	0.12				
pyrene-tetra-cyanoethylene	+	*a*	0.06 ± 0.02				111, 112
	−	*a*	0.17 ± 0.03				
naphthalene tetracyano-benzene	+	*c*	2.9 ± 0.3				113
	+	⊥*c*	4.8 ± 0.5				
anthracene tetracyano-benzene	+	*c*	2.8 ± 0.3				113
	+	⊥*c*	3.3 ± 0.3				
durene tetracyano-benzene	+	*c*	2.7 ± 0.3				113
	+	⊥*c*	3.3 ± 0.3				

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