

# Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

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Experimental values of the thermal conductivity  $\lambda$  and thermal diffusivity  $a$  of 29 pure substances are presented in the temperature range of  $-15$  °C to  $65$  °C under atmospheric or saturation pressure. The materials measured were as follows: alkenes (1-pentene, 1-hexene, 1-heptene, 1-octene, 2,3-dimethyl-1-butene, 2,3-dimethyl-2-butene), cycloalkenes (cyclopentene, cyclohexene), cycloalkanes (cyclopentane, cyclohexane, methylcyclopentane, cycloheptane, cyclooctane), aromatics and their relatives (benzene, ethylbenzene, *o*-, *m*-, and *p*-xylenes, propylbenzene, isopropylbenzene, hemimellitene, pseudocumene, mesitylene, 1,3-cyclohexadiene, 1,4-cyclohexadiene, bicyclo[2.2.1]hepta-2,5-diene [norbornadiene]), and deuterated hydrocarbons (benzene- $d_6$ , cyclohexane- $d_{12}$ , toluene- $d_8$ ). Measurements were made with the transient hot-wire method in the manner previously presented, and the thermal diffusivity values were corrected by reference to the heat capacity of heptane as a reference material. Heat capacities (volumic,  $c_{p\rho}$ ; massic,  $c_p$ ; molar,  $C_{m,p}$ ) were complementally derived from the relationship  $c_{p\rho} = \lambda/a$ , with values for the density and the molar mass. The uncertainty of the data is estimated to be 0.4% for the thermal conductivity (absolutely measured) and about 1.8% for the thermal diffusivity (with a coverage factor of  $k_p = 2$ ;  $p = 95\%$ ), although that of  $\lambda$  (not of  $a$ ) is possibly inferior for a few substances containing slightly more impurities (i.e., mainly other isomers).

## Introduction

The thermophysical transport properties of chain, branched, and cyclic hydrocarbons, with their respectively different structures, including their isomers and deuterated hydrocarbons, are important for investigating the mechanism of the conductive heat transfer on various chemical processes. The authors have previously presented their results on alkanes obtained with the transient hot-wire method.<sup>1–3</sup> In a continuation of this work, reported here are measurements of 29 hydrocarbons and deuterated compounds. The materials measured were the following:  $C_5H_8$  (cyclopentene),  $C_5H_{10}$  (1-pentene, cyclopentane),  $C_6H_6$  (benzene),  $C_6H_8$  (1,3-cyclohexadiene, 1,4-cyclohexadiene),  $C_6H_{10}$  (cyclohexene),  $C_6H_{12}$  (1-hexene, 2,3-dimethyl-1-butene, 2,3-dimethyl-2-butene, methylcyclopentane, cyclohexane),  $C_7H_8$  (bicyclo[2.2.1]hepta-2,5-diene [norbornadiene]),  $C_7H_{14}$  (1-heptene, cycloheptane),  $C_8H_{10}$  (ethylbenzene, 1,2-dimethylbenzene (*o*-xylene), 1,3-dimethylbenzene (*m*-xylene), 1,4-dimethylbenzene (*p*-xylene)),  $C_8H_{16}$  (1-octene, cyclooctane),  $C_9H_{12}$  (*n*-propylbenzene, (1-methylethyl)benzene (isopropylbenzene, cumene), 1,2,3-trimethylbenzene (hemimellitene), 1,2,4-trimethylbenzene (pseudocumene), 1,3,5-trimethylbenzene (mesitylene)), and three deuterated hydrocarbons (benzene- $d_6$ , toluene- $d_8$ , cyclohexane- $d_{12}$ ). The present paper illustrates the lists of these results in detail.

The thermal conductivity and thermal diffusivity measurements were analyzed using two temperatures,  $T_\lambda$  and  $T_a$ , which are referred to for the two measured values.<sup>3,4</sup> A small diameter is required for the wire (platinum,  $\sim 15$   $\mu\text{m}$ ) in order to derive the thermal diffusivity in the transient

hot-wire method, but its accurate determination is generally difficult. Uniformity along the axis is also needed. Therefore the calibration factors  $k_f$  are introduced for the thermal diffusivity values using the relationship  $a_{\text{ref}} = \lambda_m / c_{p\rho}$  with the volumic heat capacity value  $c_{p\rho}$  (1.5270  $\text{MJ}\cdot\text{m}^{-3}\cdot\text{K}^{-1}$ ) and the measured thermal conductivity  $\lambda_m$  at 298.15 K of heptane.<sup>4</sup> The correction or calibration factor is about 0.8–1.7% for the thermal diffusivity values calculated as  $2r = 15$   $\mu\text{m}$  in diameter, and this corresponds to the adjustments by 0.4–0.9% for the diameter of the wires.

## Measurement Procedure

**Transient Hot-Wire Method Model.** An actual model of the transient hot-wire method can be described by a transfer function having a feedback loop (i.e., the heating rate of the wire,  $q(t) = Q_0(1 + A\Delta T(t) + B\Delta T^2(t) + \dots)$ ,  $t \geq 0$ ), where  $A$  and  $B$  are fixed by the temperature dependence of the wire resistance and the circuit arrangement including the type of power supply, because the wire acts in two ways: as an electrical heating element and as a resistance thermometer. The temperature rise in the wire  $\Delta T(t)$  is fitted to the working equation, and analytically derived, with the parameters thermal conductivity  $\lambda$  and thermal diffusivity  $a$ .<sup>4,5</sup>

**Effective Temperature  $T_\lambda$  and  $T_a$  to be Referred to as  $\lambda$  and  $a$ .** In techniques such as the transient hot-wire method that involve a temperature gradient, the temperatures associated with the thermal conductivity  $\lambda$  and thermal diffusivity  $a$  values ought to be modified from  $T_0$ , which is the bath temperature or the starting temperature. Modified temperatures  $T_\lambda$  and  $T_a$  are derived from the values of the temperature dependence of the thermal conductivity and thermal diffusivity, the heating parameter

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**Table 1. List of Materials: Names (Alternative Names), Chemical Abstracts Service Registry Numbers, Formulas, Claimed Purities, and Suppliers**

name (alternative name)	CASRN	formula	purity	supplier <sup>a</sup> /lot
1-pentene	109-67-1	C <sub>5</sub> H <sub>10</sub>	98%	T.C.I./FGG01
1-hexene	592-41-6	C <sub>6</sub> H <sub>12</sub>	98%	W.P.C./ACH6692
2,3-dimethyl-1-butene	563-78-0	C <sub>6</sub> H <sub>12</sub>	98%	W.P.C./KSK5578
2,3-dimethyl-2-butene	563-79-1	C <sub>6</sub> H <sub>12</sub>	98%	A.O.U./A014156801 <sup>b</sup>
1-heptene	592-76-7	C <sub>7</sub> H <sub>14</sub>	98%	T. C. I./FIF01
1-octene	111-66-0	C <sub>8</sub> H <sub>16</sub>	99%	A.O.U./A014156301
cyclopentene	142-29-0	C <sub>5</sub> H <sub>8</sub>	97%	W.P.C./ACR2120
cyclohexene	110-83-8	C <sub>6</sub> H <sub>10</sub>	97%	W.P.C./ELP6186
cyclopentane	287-92-3	C <sub>5</sub> H <sub>10</sub>	98%	T. C. I./FHJ01
cyclohexane	110-82-7	C <sub>6</sub> H <sub>12</sub>	99.8%	W.P.C./TPF9454
cyclohexane- <i>d</i> <sub>12</sub>	1735-17-7	C <sub>6</sub> D <sub>12</sub>	99.5%	Al.C.Co./99.5% deuterium
methylcyclopentane	96-37-7	C <sub>6</sub> H <sub>12</sub>	98%	W.P.C./ACM4380
cycloheptane	291-64-5	C <sub>7</sub> H <sub>14</sub>	97%	W.P.C./ACL5336
cyclooctane	292-64-8	C <sub>8</sub> H <sub>16</sub>	98%	W.P.C./SKE5436
benzene	71-43-2	C <sub>6</sub> H <sub>6</sub>	99%	Dojin-Do/EL115
benzene- <i>d</i> <sub>6</sub>	1076-43-3	C <sub>6</sub> D <sub>6</sub>	99.6%	W.P.C./ACR7174
1,3-cyclohexadiene	592-57-4	C <sub>6</sub> H <sub>8</sub>	97%	Al.C.Co./KU12404KU <sup>c</sup>
1,4-cyclohexadiene	628-41-1	C <sub>6</sub> H <sub>8</sub>	97%	Al.C.Co./TU11510LU <sup>d</sup>
toluene- <i>d</i> <sub>8</sub>	2037-26-5	C <sub>7</sub> D <sub>8</sub>	98%	Sig.Al.Jpn./151998 <sup>e</sup>
bicyclo[2.2.1]hepta-2,5-diene (norbornadiene)	121-46-0	C <sub>7</sub> H <sub>8</sub>	98%	Al.C.Co./04902CU <sup>f</sup>
ethylbenzene	100-41-4	C <sub>8</sub> H <sub>10</sub>	98%	W.P.C./WTE4346
1,2-dimethylbenzene ( <i>o</i> -xylene)	95-47-6	C <sub>8</sub> H <sub>10</sub>	98%	W.P.C./PAP4854
1,3-dimethylbenzene ( <i>m</i> -xylene)	108-38-3	C <sub>8</sub> H <sub>10</sub>	98%	W.P.C./WTJ5486
1,4-dimethylbenzene ( <i>p</i> -xylene)	106-42-3	C <sub>8</sub> H <sub>10</sub>	98%	W.P.C./PAR4422
<i>n</i> -propylbenzene	103-65-1	C <sub>9</sub> H <sub>12</sub>	99%	T.C.I./FGG01
(1-methylethyl)-benzene(cumene)	98-82-8	C <sub>9</sub> H <sub>12</sub>	99%	T.C.I./GK01
1,2,3-trimethylbenzene (hemimellitene)	526-73-8	C <sub>9</sub> H <sub>12</sub>	95+%	W.P.C./WTP4537 <sup>g</sup>
1,2,4-trimethylbenzene (pseudocumene)	95-63-6	C <sub>9</sub> H <sub>12</sub>	98%	W.P.C./PAL5310
1,3,5-trimethylbenzene (mesitylene)	108-67-8	C <sub>9</sub> H <sub>12</sub>	97%	W.P.C./PAN5011

<sup>a</sup> T.C.I., Tolyo Chemical Industries, Ltd.; W.P.C., Wako Pure Chemical Industries, Ltd.; A.O.U., Acros Organic USA; Al.C.Co., Aldrich Chemical Co.; Dojin-Do, Dojin-Do Laboratories Jpn.; Sig.Al.Jpn., Sigma Aldrich Japan. <sup>b</sup> Stabilized with 0.05% 2,6-bis(1,1-dimethylethyl)-4-methyl-phenol (BHT, butylated hydroxytoluene). <sup>c</sup> Stabilized with 0.05% BHT. <sup>d</sup> Stabilized with ~0.1% 1,4-hydroquinone, containing ~3% benzene. <sup>e</sup> 99% deuterium atom. <sup>f</sup> Stabilized with 0.02–0.1% BHT. <sup>g</sup> (Better than 95%) tested by W.P.C. for our demand.

$Q_0/4\pi\lambda$  ( $Q_0$  is the heating rate of the wire), and the elapsed times  $t_i$  and  $t_f$  assigned to the initial and final acquisition data for each experiment.<sup>3,4</sup>

**Practical Measurement System.** The experimental system and procedure are the same as those reported previously<sup>3,4</sup> using two hot-wire sensors (4-terminal resistance, i.e., AC and BD cells). The frame of the cells was identical to the previous ones, but partly new wires (nominally,  $2r = 15 \mu\text{m}$ ) were introduced. The data sampling was carried out in the same way as previously reported. The sampling interval was 50 ms, the integrating time was always 20 ms, and the data was usually obtained in sets of 20. The elapsed times,  $t_i$  and  $t_f$  were nominally  $t_i \approx 0.03 \text{ s}$  and  $t_f \approx 1 \text{ s}$  in the present case. The set of data  $\{\Delta T(t), t_j\}$  was fitted into the nonlinear working equation using Deming's least-squares method.<sup>3,4</sup>

**Calibration Factors  $k_f$  for Thermal Diffusivity.** The data for regular configurations were designated set A for cell AC and those for an inverted position, set C; similarly, the regular position for cell BD is associated with set B and the inverted position for set D. To eliminate the systematic differences resulting from the cells and the configuration of the experiment, the data for the thermal diffusivity were adjusted by the correction factor  $k_f$ , which was based on the values of heptane,  $c_p = 2.2429 \text{ kJ}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$  and  $\rho = 679.46 \text{ kg}\cdot\text{m}^{-3}$  at 298.15 K,<sup>6,7</sup> and the relationship  $a = \lambda/c_p\rho$  (where  $\lambda_{298.15 \text{ K}}$  was determined from the results of an experiment carried out separately for calibration). The calibration factors  $k_f$  for thermal diffusivity were then introduced. Measured thermal diffusivity data were multiplied by  $k_f$  for the respective groups. These adjustments are about +1.7% for cell AC and -0.8% for cell BD. This is equivalent to an adjustment for the diameter (nominal value of  $15 \mu\text{m}$ ) of the wire by approximately +0.9% for cell AC and -0.4% for cell BD.

## Results

**Materials.** The liquid samples employed in the present measurements were obtained from various chemical product suppliers. We used them without any further purification or removal of dissolved water or air. Since some of the materials used were expensive and some are unstable, and they were stabilized with appropriate materials. The transfer of samples to the hot-wire glass tube was carried out by a syringe and a siphon after pumping to give a rough vacuum inside the sample containers so as to reduce long exposure to the atmosphere.

The list of test materials is presented in Table 1 along with Chemical Abstracts Registry Numbers (CAS RN) and formulas, together with claimed purities and their lot numbers as designated by the suppliers. The additional comments on substances are as follows: 2,3-dimethyl-2-butene is stabilized with 0.05% 2,6-bis(1,1-dimethylethyl)-4-methyl-phenol (BHT, butylated hydroxytoluene); 1,3-cyclohexadiene is stabilized with 0.05% BHT; 1,4-cyclohexadiene is stabilized with ~0.1% 1,4-hydroquinone and containing ~3% benzene; toluene-*d*<sub>8</sub> is 98% pure (99% of deuterium); bicyclo[2.2.1]hepta-2,5-diene is stabilized with 0.02–0.1%; 1,2,3-trimethylbenzene is more than 95% pure, as tested by Wako Pure Chemicals.

Specifying something mixed in the sample is important in order to accurately determine the property of a material, and also the purities claimed by manufacturers may often be over estimated. In addition, the substances of the unsaturated alkenes and dienes among the test materials seem to have been transitional to the other state due to inappropriate handling and preservation. Nevertheless, we referred to the purities indicated or claimed on the labels or catalog by the manufacturers. In fact, most of the impurities are assumed to be isomers that are difficult to separate from the sample material, because their boiling temperatures approach each other. The thermal properties

**Table 2. Experimental Data and Fitted Values (Subscript c) on Thermal Conductivity  $\lambda$  and Thermal Diffusivity  $a$  (at 0.1013 MPa) Referring to the Temperatures  $\vartheta_\lambda$  and  $\vartheta_a$** 

$\vartheta_\lambda/^\circ\text{C}$	$\vartheta_a/^\circ\text{C}$	$\lambda/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\lambda_c/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\vartheta_a/^\circ\text{C}$	$a^a/10^{-8}\text{ m}^2\cdot\text{s}^{-1}$	$a_c^a/10^{-8}\text{ m}^2\cdot\text{s}^{-1}$	$(Q_0/4\pi\lambda)/\text{K}$
1-Pentene Data (Measured with Cell AC)							
20.0101	20.8931	0.11406	0.11405	22.6479	8.202	8.201	0.1374
20.0099	21.2729	0.11394	0.11391	23.7215	8.162	8.169	0.1956
20.0101	21.5072	0.11390	0.11380	24.5198	8.163	8.146	0.2365
-16.5181	-15.7854	0.12842	0.12848	-14.2193	9.277	9.282	0.1194
-16.5187	-15.478	0.12834	0.12835	-13.2445	9.284	9.254	0.1694
-16.5183	-15.218	0.12827	0.12827	-12.5772	9.247	9.234	0.2050
2.5192	3.3237	0.12098	0.12096	4.9552	8.646	8.720	0.1283
2.5199	3.6731	0.12092	0.12082	6.0308	8.697	8.688	0.1825
2.5221	3.9179	0.12035	0.12073	6.751	8.661	8.667	0.2208
27.0481	27.9222	0.11128	0.11127	29.7289	7.993	7.993	0.1507
27.0481	28.311	0.11116	0.11112	30.836	7.958	7.960	0.2139
27.0485	28.5964	0.11110	0.11102	31.6502	7.957	7.936	0.2589
1-Hexene Data (Measured with cell AC)							
21.9217	22.6934	0.11809	0.11811	24.1855	8.252	8.226	0.1283
21.9215	23.1059	0.11777	0.11796	25.4411	8.215	8.195	0.2000
21.9199	23.3758	0.11786	0.11788	26.1771	8.197	8.177	0.2428
27.3530	28.1231	0.11609	0.11626	29.6208	8.049	8.091	0.1314
27.3530	28.5833	0.11600	0.11611	30.9273	8.065	8.058	0.2052
27.3530	28.8109	0.11577	0.11602	31.6560	8.042	8.040	0.2481
-13.9076	-13.2231	0.13039	0.13032	-11.9054	9.120	9.126	0.1096
-13.9068	-12.9555	0.13048	0.13022	-11.0184	9.145	9.104	0.1570
-13.9069	-12.6761	0.13028	0.13012	-10.1062	9.138	9.081	0.2060
2.1201	2.8305	0.12475	0.12485	4.2331	8.631	8.724	0.1202
2.1221	3.1300	0.12492	0.12475	5.1463	8.692	8.701	0.1693
2.1219	3.4488	0.12452	0.12464	6.0956	8.669	8.677	0.2225
40.7295	41.5165	0.11186	0.11170	43.0607	7.674	7.756	0.1395
40.7297	41.8900	0.11148	0.11158	44.1155	7.707	7.730	0.2001
40.7298	42.2309	0.11119	0.11146	45.1628	7.677	7.704	0.2634
55.1304	55.9859	0.10713	0.10679	57.6131	7.418	7.393	0.1483
55.1311	56.3759	0.10700	0.10666	58.6637	7.391	7.367	0.2122
55.1313	56.7428	0.10683	0.10653	59.8084	7.397	7.339	0.2792
2,3-Dimethyl-1-butene (Measured with Cell BD)							
20.1852	21.0287	0.10578	0.10599	22.5000	7.300	7.332	0.1550
20.1856	21.3830	0.10561	0.10588	23.5344	7.294	7.309	0.2193
20.1853	21.6323	0.10551	0.10581	24.2280	7.277	7.293	0.2655
4.3507	5.1429	0.11075	0.11084	6.5839	7.655	7.707	0.1439
4.3511	5.4817	0.11064	0.11074	7.5506	7.674	7.684	0.2042
4.3505	5.7224	0.11055	0.11066	8.2392	7.679	7.668	0.2473
-14.9164	-14.1742	0.11700	0.11674	-12.7850	8.168	8.161	0.1317
-14.9173	-13.8584	0.11687	0.11664	-11.8641	8.189	8.139	0.1869
-14.9170	-13.7506	0.11679	0.11661	-11.6000	8.160	8.132	0.2070
38.8144	39.7108	0.10021	0.10029	41.2840	6.879	6.892	0.1672
38.8154	40.0830	0.10001	0.10018	42.2973	6.843	6.869	0.2375
38.8151	40.3493	0.09991	0.10010	43.0273	6.831	6.852	0.2877
52.4312	53.3667	0.09639	0.09612	54.9845	6.580	6.571	0.1767
52.4309	53.7624	0.09621	0.09600	56.0653	6.585	6.546	0.2511
52.4309	54.0581	0.09612	0.09591	56.9017	6.621	6.526	0.3040
48.4457	49.3582	0.09740	0.09735	50.9174	6.600	6.666	0.1743
48.4456	49.7550	0.09730	0.09723	52.0222	6.650	6.641	0.2469
48.4457	50.0254	0.09720	0.09714	52.7486	6.622	6.624	0.2992
2,3-Dimethyl-2-butene Data (Measured with cell AC)							
20.1858	20.9399	0.12276	0.12289	22.3368	8.480	8.456	0.1350
20.1851	21.2514	0.12257	0.12278	23.2173	8.436	8.432	0.1922
20.1859	21.4799	0.12249	0.12270	23.8733	8.446	8.414	0.2326
4.3526	5.0614	0.12853	0.12855	6.3903	8.879	8.892	0.1262
4.3522	5.3550	0.12835	0.12845	7.2303	8.850	8.869	0.1789
4.3514	5.5684	0.12827	0.12837	7.8492	8.855	8.852	0.2167
-14.9188	-14.2628	0.13562	0.13543	-13.0141	9.383	9.423	0.1155
-14.9182	-13.9811	0.13548	0.13533	-12.1853	9.413	9.400	0.1640
-14.9176	-13.7833	0.13540	0.13526	-11.6089	9.410	9.384	0.1980
38.8132	39.6128	0.11621	0.11624	41.0547	7.956	7.945	0.1466
38.8071	39.9448	0.11604	0.11612	42.0003	7.951	7.919	0.2083
38.8091	40.1859	0.11595	0.11603	42.6732	7.944	7.900	0.2521
52.4313	53.2655	0.11163	0.11137	54.7433	7.601	7.570	0.1552
52.4311	53.6233	0.11149	0.11125	55.7498	7.626	7.543	0.2203
52.4309	53.8676	0.11137	0.11116	56.4174	7.592	7.525	0.2668
48.4457	49.2542	0.11279	0.11280	50.6626	7.580	7.682	0.1531
48.4458	49.5908	0.11258	0.11268	51.5823	7.557	7.657	0.2171
48.4459	49.8304	0.11248	0.11260	52.2356	7.544	7.639	0.2629
1-Heptene Data (Measured with Cell AC)							
23.4391	24.2134	0.12130	0.12154	25.7358	8.275	8.298	0.1374
23.4383	24.5642	0.12127	0.12144	26.7171	8.268	8.275	0.1956
23.4388	24.7987	0.12117	0.12136	27.3958	8.253	8.259	0.2365
-11.3927	-10.6927	0.13253	0.13248	-9.3189	9.064	9.105	0.1194
-11.3932	-10.3957	0.13238	0.13238	-8.4101	9.110	9.084	0.1694
-11.3925	-10.1813	0.13237	0.13232	-7.7828	9.101	9.069	0.2050
6.5891	7.3348	0.12684	0.12683	8.7804	8.665	8.688	0.1283
6.5895	7.6535	0.12671	0.12673	9.7230	8.674	8.666	0.1825
6.5897	7.8769	0.12638	0.12666	10.3809	8.662	8.651	0.2208
46.4710	47.3237	0.11445	0.11431	48.9165	7.761	7.764	0.1507
46.4701	47.6817	0.11430	0.11420	49.9484	7.757	7.740	0.2139
46.4697	47.9327	0.11416	0.11412	50.6614	7.731	7.724	0.2589

Table 2. (Continued)

$\vartheta_0/^\circ\text{C}$	$\vartheta_2/^\circ\text{C}$	$\lambda/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\lambda_c/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\vartheta_d/^\circ\text{C}$	$a^a/10^{-8}\text{m}^2\cdot\text{s}^{-1}$	$a_c^a/10^{-8}\text{m}^2\cdot\text{s}^{-1}$	$(Q_0/4\pi\lambda)/\text{K}$
1-Octene Data (Measured with Cell AC)							
23.2101	23.7277	0.12400	0.12425	24.5000	7.980	8.063	0.1350
23.2101	23.9924	0.12404	0.12417	25.1261	7.997	8.046	0.1985
23.2092	24.1258	0.12402	0.12413	25.4589	8.018	8.037	0.2310
-13.9636	-13.4613	0.13536	0.13528	-12.6858	9.041	9.023	0.1163
-13.9642	-13.2456	0.13531	0.13522	-12.1297	9.074	9.008	0.1649
-13.9641	-13.0914	0.13525	0.13517	-11.7323	9.089	8.998	0.1993
5.6843	6.1895	0.12942	0.12945	6.9333	8.389	8.516	0.1257
5.6846	6.4168	0.12937	0.12938	7.5093	8.475	8.501	0.1780
5.6823	6.5729	0.12900	0.12934	7.9100	8.490	8.491	0.2150
42.1337	42.6717	0.11847	0.11863	43.4243	7.494	7.573	0.1447
42.1334	42.9205	0.11856	0.11856	44.0384	7.584	7.557	0.2050
42.1337	43.0927	0.11855	0.11851	44.4607	7.610	7.546	0.2476
52.7453	53.2855	0.11549	0.11548	54.0276	7.236	7.299	0.1502
52.7452	53.5461	0.11556	0.11541	54.6686	7.347	7.282	0.2125
52.7452	53.7248	0.11556	0.11535	55.1052	7.380	7.271	0.2572
Cyclopentene Data (Measured with Cell AC)							
21.1770	21.7658	0.13302	0.13319	22.7319	9.782	9.796	0.1250
21.1769	22.0144	0.13284	0.13308	23.3915	9.784	9.770	0.1774
21.1755	22.1850	0.13272	0.13301	23.8381	9.744	9.752	0.2151
3.2870	3.8433	0.14087	0.14094	4.7814	10.467	10.515	0.1149
3.2874	4.0798	0.14066	0.14084	5.4194	10.467	10.489	0.1632
3.2878	4.2459	0.14056	0.14077	5.8656	10.457	10.471	0.1973
-14.9581	-14.4299	0.14913	0.14884	-13.5080	11.252	11.247	0.1052
-14.9579	-14.2086	0.14887	0.14875	-12.8990	11.241	11.222	0.1490
-14.9581	-14.0497	0.14879	0.14868	-12.4608	11.238	11.205	0.1800
38.8194	39.4302	0.12584	0.12555	40.3961	9.094	9.089	0.1354
38.8200	39.6883	0.12563	0.12544	41.0625	9.083	9.062	0.1923
38.8201	39.8661	0.12552	0.12536	41.5162	9.050	9.044	0.2329
Cyclohexene Data (Measured with Cell AC)							
22.6166	23.1270	0.12783	0.12797	23.8759	8.878	8.905	0.1306
22.6154	23.3391	0.12768	0.12790	24.4023	8.872	8.889	0.1850
22.6171	23.4976	0.12759	0.12785	24.7937	8.880	8.877	0.2241
-16.4081	-15.9288	0.14059	0.14050	-15.1780	10.124	10.102	0.1113
-16.4084	-15.7279	0.14045	0.14044	-14.6602	10.121	10.086	0.1577
-16.4086	-15.5836	0.14038	0.14039	-14.2880	10.121	10.075	0.1909
1.7246	2.2199	0.13476	0.13468	2.9735	9.551	9.546	0.1199
1.7219	2.4257	0.13461	0.13461	3.4981	9.551	9.530	0.1699
1.7223	2.5778	0.13458	0.13456	3.8845	9.562	9.518	0.2058
37.9916	38.5169	0.12308	0.12303	39.2728	8.465	8.433	0.1385
37.9916	38.7372	0.12293	0.12296	39.8110	8.457	8.416	0.1964
37.9913	38.8878	0.12279	0.12291	40.1750	8.423	8.405	0.2378
54.1674	54.6968	0.11801	0.11784	55.4371	7.972	7.937	0.1471
54.1670	54.9211	0.11784	0.11777	55.9777	7.974	7.921	0.2086
54.1675	55.0742	0.11773	0.11772	56.3408	7.941	7.910	0.2529
21.9210	22.4163	0.12840	0.12820	23.1357	8.828	8.928	0.1298
21.9202	22.6161	0.12817	0.12813	23.6231	8.777	8.913	0.1841
21.9200	22.7671	0.12811	0.12809	23.9957	8.788	8.901	0.2231
Cyclopentane Data (Measured with Cell BD)							
20.0096	20.4840	0.12811	0.12815	21.1798	9.638	9.618	0.1275
20.0098	20.6819	0.12791	0.12807	21.6679	9.616	9.597	0.1809
20.0098	20.8240	0.12781	0.12802	22.0184	9.607	9.583	0.2192
-16.5175	-16.0721	0.14283	0.14257	-15.3749	11.145	11.144	0.1075
-16.5175	-15.8825	0.14263	0.14250	-14.8859	11.148	11.124	0.1526
-16.5172	-15.7515	0.14252	0.14245	-14.5515	11.121	11.110	0.1847
2.5249	2.9837	0.13495	0.13506	3.6755	10.301	10.349	0.1178
2.5250	3.1759	0.13480	0.13498	4.1569	10.280	10.328	0.1674
2.5252	3.3222	0.13479	0.13492	4.5320	10.341	10.313	0.2020
27.0484	27.5180	0.12539	0.12538	28.1942	9.297	9.325	0.1316
27.0485	27.7159	0.12525	0.12530	28.6777	9.294	9.304	0.1866
27.0484	27.8553	0.12514	0.12524	29.0176	9.278	9.290	0.2261
42.5858	43.0576	0.11948	0.11925	43.7178	8.682	8.676	0.1411
42.5861	43.2550	0.11931	0.11917	44.1911	8.665	8.657	0.2003
42.5859	43.3921	0.11922	0.11911	44.5198	8.649	8.643	0.2422
Cyclohexane Data (Measured with Cell BD)							
27.3093	27.6893	0.11746	0.11740	28.2032	8.091	8.121	0.1405
27.3095	27.8477	0.11729	0.11735	28.5758	8.061	8.110	0.2007
27.3092	27.9908	0.11725	0.11731	28.9134	8.090	8.099	0.2504
7.2894	7.6847	0.12318	0.12312	8.2308	8.754	8.736	0.1299
7.2892	7.8522	0.12309	0.12307	8.6302	8.734	8.723	0.1850
7.2900	7.9959	0.12298	0.12303	8.9722	8.753	8.713	0.2317
21.9968	22.3786	0.11898	0.11892	22.8970	8.246	8.284	0.1377
21.9973	22.5498	0.11887	0.11887	23.3012	8.280	8.272	0.1956
21.9971	22.6827	0.11874	0.11883	23.6145	8.244	8.262	0.2456
45.1375	45.5122	0.11242	0.11231	46.0141	7.599	7.573	0.1504
45.1380	45.6712	0.11226	0.11226	46.3859	7.589	7.562	0.2138
45.1368	45.7983	0.11215	0.11222	46.6857	7.561	7.552	0.2683

Table 2. (Continued)

$\vartheta_0/^\circ\text{C}$	$\vartheta_2/^\circ\text{C}$	$\lambda/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\lambda_c/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\vartheta_d/^\circ\text{C}$	$a^a/10^{-8}\text{m}^2\cdot\text{s}^{-1}$	$a_c^a/10^{-8}\text{m}^2\cdot\text{s}^{-1}$	$(Q_0/4\pi\lambda)/\text{K}$
Cyclohexane- $d_{12}$ Data (Measured with Cell BD)							
6.9288	7.3126	0.11631	0.11615	7.8156	6.835	6.807	0.1376
6.9289	7.4784	0.11619	0.11611	8.1996	6.846	6.797	0.1952
6.9286	7.5861	0.11606	0.11608	8.4482	6.814	6.791	0.2364
17.6628	18.0283	0.11331	0.11331	18.5032	6.504	6.550	0.1437
17.6627	18.1942	0.11327	0.11326	18.8851	6.539	6.541	0.2043
17.6624	18.3030	0.11317	0.11324	19.1361	6.529	6.535	0.2467
30.1625	30.5230	0.11001	0.10999	30.9899	6.225	6.251	0.1509
30.1629	30.6777	0.10987	0.10995	31.3442	6.223	6.242	0.2145
30.1627	30.7735	0.10976	0.10993	31.5657	6.192	6.237	0.2588
42.4142	42.7551	0.10667	0.10675	43.1993	5.907	5.958	0.1579
42.4148	42.9121	0.10663	0.10670	43.5576	5.935	5.949	0.2247
42.4144	43.0238	0.10660	0.10667	43.8134	5.955	5.943	0.2710
52.8003	53.1468	0.10422	0.10399	53.5976	5.751	5.708	0.1638
52.8000	53.2899	0.10400	0.10395	53.9280	5.732	5.700	0.2328
52.8002	53.3882	0.10397	0.10392	54.1554	5.721	5.695	0.2816
Methylcyclopentane Data (Measured with Cell BD)							
21.1749	21.7522	0.11555	0.11558	22.6085	8.242	8.281	0.1416
21.1749	21.9971	0.11540	0.11550	23.2193	8.245	8.263	0.2009
21.1745	22.1700	0.11532	0.11544	23.6500	8.236	8.250	0.2434
3.2875	3.8492	0.12118	0.12127	4.7103	8.804	8.827	0.1315
3.2881	4.0937	0.12109	0.12120	5.3388	8.845	8.808	0.1862
3.2865	4.2587	0.12100	0.12114	5.7580	8.821	8.795	0.2256
-14.9577	-14.4437	0.12729	0.12710	-13.6295	9.396	9.387	0.1154
-14.9574	-14.1938	0.12711	0.12702	-12.9857	9.368	9.367	0.1719
-14.9574	-14.0361	0.12701	0.12697	-12.5814	9.343	9.355	0.2081
38.8230	39.4232	0.11013	0.10995	40.2918	7.769	7.742	0.1522
38.8226	39.6685	0.10995	0.10987	40.8879	7.729	7.724	0.2162
38.8228	39.8431	0.10986	0.10982	41.3126	7.714	7.711	0.2614
Cycloheptane Data (Measured with Cell BD)							
23.4385	23.8637	0.11869	0.11868	24.4413	7.965	8.013	0.1388
23.4390	24.0482	0.11853	0.11864	24.8777	7.978	8.003	0.1970
23.4395	24.1776	0.11848	0.11861	25.1833	7.982	7.995	0.2378
-11.3925	-10.9719	0.12721	0.12715	-10.3769	8.837	8.868	0.1222
-11.3924	-10.7823	0.12714	0.12711	-9.9122	8.903	8.856	0.1733
-11.3916	-10.6516	0.12706	0.12708	-9.5944	8.912	8.848	0.2091
6.5918	7.0170	0.12282	0.12278	7.6058	8.389	8.426	0.1306
6.5913	7.1968	0.12273	0.12274	8.0368	8.396	8.416	0.1851
6.5898	7.3252	0.12268	0.12271	8.3469	8.403	8.408	0.2239
46.4700	46.8986	0.11322	0.11308	47.4700	7.466	7.448	0.1496
46.4697	47.0817	0.11307	0.11304	47.8982	7.465	7.438	0.2126
46.4704	47.2085	0.11298	0.11301	48.1934	7.456	7.430	0.2568
Cyclooctane Data (Measured with Cell AC)							
22.2734	22.6951	0.11910	0.11892	23.2841	7.395	7.364	0.1153
22.2732	22.9391	0.11888	0.11890	23.8667	7.359	7.359	0.1835
22.2729	23.0569	0.11882	0.11886	24.1495	7.357	7.351	0.2158
22.2726	22.7271	0.11910	0.11888	23.3584	7.352	7.356	0.1261
15.0864	15.5469	0.12047	0.12045	16.1920	7.481	7.497	0.1256
15.0853	15.8057	0.12030	0.12039	16.8175	7.485	7.485	0.1955
15.0857	16.0204	0.12023	0.12035	17.3347	7.485	7.476	0.2531
38.0051	38.5200	0.11560	0.11554	39.2222	7.054	7.067	0.1480
38.0070	38.7343	0.11543	0.11550	39.7243	7.027	7.058	0.2104
38.0067	38.9544	0.11536	0.11545	40.2473	7.037	7.048	0.2726
55.3208	55.8444	0.11193	0.11184	56.5459	6.754	6.744	0.1561
55.3205	56.0663	0.11181	0.11179	57.0663	6.752	6.734	0.2217
55.3208	56.2807	0.11166	0.11175	57.5650	6.722	6.725	0.2878
Benzene Data (Measured with Cell AC)							
27.3094	28.0973	0.13987	0.13980	29.8705	9.293	9.329	0.1200
27.3092	28.4358	0.13975	0.13969	30.9821	9.308	9.306	0.1711
27.3090	28.7158	0.13956	0.13960	31.8950	9.294	9.287	0.2137
7.2900	8.0274	0.14637	0.14634	9.7096	9.740	9.752	0.1113
7.2896	8.3430	0.14620	0.14623	10.7513	9.742	9.730	0.1587
7.2896	8.6053	0.14609	0.14615	11.6049	9.715	9.713	0.1987
21.9952	22.7710	0.14156	0.14154	24.5207	9.400	9.442	0.1180
21.9960	23.1047	0.14142	0.14143	25.6268	9.443	9.418	0.1676
21.9957	23.3806	0.14133	0.14134	26.5345	9.441	9.399	0.2092
45.1479	45.9902	0.13402	0.13398	47.8882	8.973	8.951	0.1281
45.1455	46.3361	0.13382	0.13387	49.0022	8.921	8.928	0.1820
45.1437	46.6356	0.13371	0.13377	49.9678	8.896	8.908	0.2284
Benzene- $d_6$ Data (Measured with Cell AC)							
6.9302	7.6127	0.13976	0.13980	8.9407	8.096	8.158	0.1166
6.9281	7.9053	0.13973	0.13970	9.8329	8.154	8.140	0.1650
6.9287	8.1105	0.13959	0.13964	10.4330	8.124	8.129	0.2002
17.6632	18.3766	0.13645	0.13636	19.7663	7.931	7.947	0.1216
17.6637	18.6807	0.13632	0.13626	20.6751	7.956	7.929	0.1724
17.6637	18.8936	0.13624	0.13620	21.3070	7.952	7.917	0.2084
30.1609	30.9048	0.13234	0.13236	32.3438	7.696	7.702	0.1274
30.1617	31.2206	0.13221	0.13226	33.2723	7.695	7.684	0.1811
30.1610	31.4419	0.13212	0.13219	33.9266	7.694	7.671	0.2188
42.4105	43.1853	0.12842	0.12844	44.6697	7.458	7.461	0.1336
42.4111	43.5117	0.12830	0.12834	45.6206	7.450	7.443	0.1897
42.4117	43.7409	0.12820	0.12826	46.2886	7.445	7.430	0.2291
52.8005	53.5978	0.12523	0.12512	55.1086	7.250	7.258	0.1386
52.8006	53.9301	0.12505	0.12501	56.0654	7.227	7.239	0.1967
52.8004	54.1631	0.12491	0.12494	56.7308	7.203	7.226	0.2380

Table 2. (Continued)

$\vartheta_0/^\circ\text{C}$	$\vartheta_1/^\circ\text{C}$	$\lambda/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\lambda_c/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\vartheta_d/^\circ\text{C}$	$a^a/10^{-8}\text{m}^2\cdot\text{s}^{-1}$	$a_c^a/10^{-8}\text{m}^2\cdot\text{s}^{-1}$	$(Q_0/4\pi\lambda)/\text{K}$
1,3-Cyclohexadiene Data (Measured with Cell AC)							
22.4986	23.1008	0.13336	0.13310	24.0927	8.953	8.978	0.1251
22.4983	23.3593	0.13323	0.13302	24.7859	8.979	8.961	0.1776
22.4985	23.5403	0.13315	0.13297	25.2676	8.976	8.949	0.2147
40.1668	40.7971	0.12776	0.12769	41.8138	8.512	8.545	0.1338
40.1661	41.0656	0.12763	0.12761	42.5224	8.526	8.527	0.1899
40.1672	41.2553	0.12751	0.12755	43.0166	8.514	8.515	0.2298
54.7574	55.4133	0.12325	0.12322	56.4548	8.170	8.187	0.1413
54.7578	55.6886	0.12311	0.12314	57.1685	8.168	8.169	0.2002
54.7575	55.9263	0.12305	0.12307	57.8432	8.189	8.153	0.2422
5.7011	6.0195	0.13801	0.13832	6.4405	7.363		0.1179
5.7010	6.1649	0.13790	0.13828	6.7795	7.405		0.1676
5.7013	6.2646	0.13778	0.13825	7.0113	7.410		0.2024
-8.8032	-8.4861	0.14277	0.14276	-8.0623	7.718		0.1113
-8.8020	-8.3489	0.14257	0.14271	-7.7427	7.725		0.1577
-8.8024	-8.2616	0.14244	0.14269	-7.5392	7.685		0.1910
-15.1870	-14.8034	0.14507	0.14469	-14.2633	8.415		0.1081
-15.1876	-14.6345	0.14491	0.14464	-13.8516	8.449		0.1538
-15.1864	-14.5250	0.14479	0.14460	-13.5917	8.413		0.1856
1,4-Cyclohexadiene Data (Measured with Cell BD)							
22.4984	23.0532	0.14553	0.14542	23.9926	9.505	9.492	0.1126
22.4986	23.2820	0.14526	0.14534	24.6013	9.448	9.475	0.1602
22.4987	23.4464	0.14519	0.14528	25.0431	9.445	9.462	0.1937
40.1668	40.7470	0.13934	0.13926	41.7054	9.009	8.995	0.1208
40.1669	40.9845	0.13903	0.13918	42.3283	8.954	8.978	0.1714
40.1669	41.1557	0.13902	0.13912	42.7810	8.951	8.965	0.2073
54.7575	55.3569	0.13427	0.13417	56.3278	8.612	8.586	0.1274
54.7577	55.6019	0.13413	0.13409	56.9639	8.574	8.568	0.1804
54.7576	55.7807	0.13399	0.13403	57.4310	8.567	8.555	0.2186
5.7009	6.2299	0.15142	0.15127	7.1424	9.954	9.964	0.1055
5.7017	6.4524	0.15124	0.15120	7.7459	9.931	9.947	0.1500
5.7021	6.6108	0.15113	0.15114	8.1767	9.923	9.935	0.1815
-8.8030	-8.2943	0.15639	0.15633	-7.4009	10.359	10.371	0.0996
-8.8018	-8.0747	0.15627	0.15625	-6.7924	10.375	10.354	0.1417
-8.8019	-7.9236	0.15622	0.15620	-6.3757	10.364	10.343	0.1714
-15.1872	-14.6850	0.15862	0.15855	-13.7936	10.560	10.550	0.0973
-15.1863	-14.4765	0.15837	0.15848	-13.2194	10.523	10.534	0.1379
-15.1874	-14.3261	0.15834	0.15843	-12.7958	10.542	10.523	0.1667
Toluene- $d_6$ Data (Measured with Cell BD)							
23.2096	23.7475	0.12512	0.12504	24.5364	7.516	7.547	0.1313
23.2099	23.9758	0.12494	0.12498	25.1013	7.514	7.535	0.1864
23.2082	24.1337	0.12485	0.12494	25.4937	7.506	7.527	0.2254
-13.9643	-13.4616	0.13495	0.13492	-12.6844	8.330	8.339	0.1144
-13.9638	-13.2427	0.13483	0.13487	-12.1194	8.365	8.327	0.1624
-13.9639	-13.0915	0.13476	0.13483	-11.7323	8.359	8.318	0.1965
5.6815	6.2034	0.12982	0.12970	6.9881	7.896	7.920	0.1233
5.6835	6.4247	0.12970	0.12964	7.5413	7.899	7.909	0.1745
5.6829	6.5788	0.12959	0.12960	7.9268	7.881	7.900	0.2115
42.1341	42.6948	0.12002	0.12001	43.5007	7.149	7.144	0.1404
42.1339	42.9266	0.11990	0.11995	44.0637	7.128	7.132	0.1993
42.1341	43.0898	0.11979	0.11990	44.4592	7.112	7.124	0.2409
52.7449	53.3162	0.11731	0.11719	54.1275	6.951	6.918	0.1453
52.7452	53.5539	0.11718	0.11713	54.7000	6.929	6.906	0.2065
52.7449	53.7192	0.11700	0.11708	55.0966	6.904	6.898	0.2501
Bicyclo[2.2.1]hepta-2,5-diene (Norbornadiene) Data (Measured with Cell AC)							
22.8098	23.0795	0.13708	0.13678	23.4605	9.432	9.487	0.1216
22.8098	23.1969	0.13695	0.13675	23.7427	9.444	9.477	0.1726
22.8092	23.2817	0.13684	0.13672	23.9475	9.451	9.470	0.2090
-14.8803	-14.5811	0.14849	0.14858	-14.1555	10.792	10.824	0.1054
-14.8798	-14.4472	0.14844	0.14854	-13.8304	10.842	10.813	0.1495
-14.8799	-14.3527	0.14838	0.14851	-13.6003	10.853	10.804	0.1812
3.3216	3.6275	0.14263	0.14287	4.0580	10.237	10.177	0.1138
3.3210	3.7371	0.14302	0.14284	4.3232	10.175	10.167	0.1603
3.3211	3.8163	0.14289	0.14282	4.5139	10.120	10.161	0.1943
39.8627	40.1164	0.13152	0.13145	40.4805	8.845	8.882	0.1298
39.8658	40.2304	0.13142	0.13141	40.7524	8.860	8.873	0.1840
39.8680	40.3113	0.13132	0.13139	40.9452	8.860	8.866	0.2227
58.4225	58.6558	0.12564	0.12564	59.0031	8.252	8.224	0.1388
58.4235	58.7559	0.12547	0.12561	59.2502	8.247	8.215	0.1969
58.4237	58.8253	0.12539	0.12559	59.4230	8.238	8.209	0.2386
Ethylbenzene Data (Measured with Cell AC)							
21.9204	22.7052	0.12816	0.12809	24.2912	8.657	8.664	0.1300
21.9203	23.0366	0.12804	0.12801	25.3014	8.670	8.643	0.1844
21.9198	23.2700	0.12797	0.12795	26.0077	8.658	8.628	0.2231
3.4435	4.1903	0.13283	0.13271	5.7295	9.038	9.048	0.1219
3.4436	4.5032	0.13270	0.13263	6.6859	9.023	9.028	0.1731
3.4436	4.7273	0.13262	0.13257	7.3753	9.024	9.014	0.2094
-15.8624	-15.1535	0.13753	0.13753	-13.6594	9.446	9.450	0.1137
-15.8629	-14.8572	0.13738	0.13745	-12.7369	9.434	9.431	0.1614
-15.8634	-14.6472	0.13728	0.13740	-12.0884	9.412	9.417	0.1954
38.4119	39.2267	0.12395	0.12398	40.8352	8.290	8.321	0.1375
38.4123	39.5696	0.12383	0.12389	41.8563	8.284	8.300	0.1951
38.4121	39.8113	0.12375	0.12383	42.5764	8.279	8.285	0.2359
55.0512	55.8990	0.11986	0.11982	57.5436	7.966	7.975	0.1450
55.0508	56.2562	0.11974	0.11974	58.5949	7.959	7.953	0.2061
55.0515	56.5089	0.11964	0.11967	59.3373	7.953	7.938	0.2491

Table 2. (Continued)

$\vartheta_0/^\circ\text{C}$	$\vartheta_2/^\circ\text{C}$	$\lambda/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\lambda_c/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\vartheta_d/^\circ\text{C}$	$a^a/10^{-8}\text{m}^2\cdot\text{s}^{-1}$	$a_c^a/10^{-8}\text{m}^2\cdot\text{s}^{-1}$	$(Q_0/4\pi\lambda)/\text{K}$
1,2-Dimethylbenzene ( <i>o</i> -Xylene) Data (Measured with Cell BD)							
21.9195	22.4148	0.12964	0.12927	23.1402	8.464	8.464	0.1264
21.9198	22.6262	0.12957	0.12922	23.6647	8.482	8.454	0.1792
21.9201	22.7641	0.12937	0.12920	23.9968	8.420	8.448	0.2171
3.4442	3.9228	0.13341	0.13313	4.6351	8.779	8.813	0.1194
3.4443	4.1207	0.13326	0.13309	5.1252	8.751	8.803	0.1695
3.4443	4.2710	0.13327	0.13306	5.5065	8.794	8.796	0.2048
-15.8635	-15.3960	0.13684	0.13717	-14.6843	9.156	9.177	0.1124
-15.8632	-15.1893	0.13687	0.13713	-14.1521	9.207	9.166	0.1592
-15.8627	-15.0482	0.13677	0.13710	-13.7959	9.189	9.160	0.1929
38.4121	38.9249	0.12591	0.12582	39.6666	8.182	8.153	0.1331
38.4120	39.1379	0.12583	0.12577	40.1880	8.171	8.143	0.1886
38.4125	39.2865	0.12572	0.12574	40.5473	8.150	8.136	0.2286
55.0512	55.5697	0.12219	0.12234	56.3036	7.831	7.840	0.1399
55.0511	55.7884	0.12201	0.12229	56.8328	7.826	7.830	0.1985
55.0513	55.9406	0.12193	0.12226	57.1984	7.808	7.823	0.2404
1,3-Dimethylbenzene ( <i>m</i> -Xylene) Data (Measured with Cell AC)							
20.3376	20.9184	0.13055	0.13044	21.8428	9.030	9.037	0.1273
20.3368	21.1656	0.13047	0.13038	22.4914	9.055	9.022	0.1804
20.3377	21.3387	0.13036	0.13034	22.9375	9.035	9.013	0.2185
13.6365	14.2070	0.13227	0.13212	15.1193	9.159	9.185	0.1245
13.6361	14.4513	0.13216	0.13206	15.7621	9.187	9.170	0.1766
13.6361	14.6216	0.13204	0.13202	16.2042	9.168	9.161	0.2139
-15.4942	-14.9845	0.13931	0.13941	-14.1424	9.793	9.828	0.1072
-15.4938	-14.7347	0.13914	0.13935	-13.4789	9.786	9.813	0.1595
-15.4935	-14.5692	0.13911	0.13930	-13.0324	9.815	9.804	0.1929
1.3340	1.8921	0.13534	0.13519	2.8009	9.458	9.455	0.1192
1.3352	2.1265	0.13526	0.13514	3.4156	9.453	9.442	0.1690
1.3332	2.2908	0.13516	0.13509	3.8499	9.438	9.432	0.2047
37.9885	38.5919	0.12605	0.12603	39.5343	8.652	8.648	0.1351
37.9912	38.8498	0.12594	0.12597	40.1944	8.659	8.633	0.1915
37.9921	39.0292	0.12584	0.12592	40.6505	8.638	8.623	0.2320
55.0172	55.6381	0.12179	0.12177	56.5872	8.276	8.273	0.1426
55.0175	55.8898	0.12162	0.12171	57.2147	8.222	8.259	0.2024
55.0176	56.0740	0.12152	0.12167	57.6794	8.217	8.249	0.2450
1,4-Dimethylbenzene ( <i>p</i> -Xylene) Data (Measured with Cell BD)							
20.3363	20.8782	0.12785	0.12784	21.7055	8.779	8.797	0.1278
20.3370	21.1203	0.12778	0.12778	22.3300	8.816	8.784	0.1813
20.3368	21.2854	0.12772	0.12773	22.7510	8.815	8.774	0.2194
13.6360	14.1828	0.12961	0.12954	15.0359	8.957	8.945	0.1248
13.6347	14.4013	0.12949	0.12948	15.5885	8.891	8.932	0.1772
13.6361	14.5759	0.12941	0.12944	16.0433	8.920	8.922	0.2144
37.9931	38.5590	0.12343	0.12335	39.4104	8.411	8.406	0.1356
37.9928	38.7918	0.12323	0.12329	39.9910	8.378	8.393	0.1925
37.9929	38.9583	0.12311	0.12325	40.4051	8.358	8.384	0.2332
55.0177	55.5986	0.11909	0.11902	56.4538	8.029	8.029	0.1434
55.0173	55.8421	0.11897	0.11896	57.0574	8.024	8.016	0.2034
55.0174	56.0143	0.11890	0.11891	57.4817	8.010	8.007	0.2465
<i>n</i> -Propylbenzene Data (Measured with Cell AC)							
20.4402	21.0221	0.12857	0.12860	21.9332	8.493	8.490	0.1292
20.4415	21.2749	0.12851	0.12854	22.5887	8.530	8.478	0.1833
20.4418	21.4495	0.12845	0.12850	23.0374	8.520	8.470	0.2219
1.3852	1.9409	0.13296	0.13277	2.8253	8.836	8.843	0.1213
1.3868	2.1828	0.13283	0.13272	3.4584	8.869	8.831	0.1722
1.3866	2.3464	0.13275	0.13268	3.8803	8.845	8.823	0.2084
-12.5096	-11.9738	0.13576	0.13581	-11.1139	9.044	9.100	0.1160
-12.5094	-11.7460	0.13567	0.13577	-10.5152	9.065	9.089	0.1643
-12.5095	-11.5840	0.13558	0.13573	-10.0906	9.061	9.081	0.1991
38.7886	39.3874	0.12468	0.12458	40.3042	8.143	8.151	0.1367
38.7897	39.6430	0.12456	0.12452	40.9541	8.157	8.139	0.1938
38.7895	39.8226	0.12452	0.12448	41.4094	8.148	8.131	0.2348
55.7732	56.3855	0.12082	0.12086	57.3016	7.798	7.838	0.1440
55.7734	56.6407	0.12074	0.12080	57.9381	7.791	7.826	0.2040
55.7732	56.8302	0.12069	0.12076	58.4173	7.809	7.817	0.2472
(1-Methylethyl)-benzene (Cumene, Isopropylbenzene) Data (Measured with Cell BD)							
20.4419	20.9591	0.12022	0.11992	21.6998	7.919	7.866	0.1359
20.4421	21.1667	0.12002	0.11988	22.1987	7.862	7.857	0.1930
20.4409	21.3204	0.11994	0.11985	22.5745	7.862	7.850	0.2337
1.3869	1.8809	0.12383	0.12371	2.5960	8.183	8.212	0.1281
1.3868	2.0938	0.12374	0.12367	3.1224	8.207	8.202	0.1817
1.3871	2.2471	0.12369	0.12364	3.5012	8.217	8.196	0.2200
-12.5094	-12.0225	0.12634	0.12647	-11.3050	8.445	8.464	0.1225
-12.5094	-11.8169	0.12624	0.12643	-10.7945	8.447	8.454	0.1737
-12.5088	-11.6712	0.12620	0.12640	-10.4349	8.439	8.448	0.2103
38.7900	39.3081	0.11636	0.11628	40.0287	7.509	7.534	0.1441
38.7899	39.5321	0.11632	0.11624	40.5692	7.537	7.525	0.2043
38.7902	39.6882	0.11622	0.11620	40.9429	7.527	7.518	0.2474
55.7736	56.3019	0.11281	0.11291	57.0245	7.207	7.227	0.1516
55.7735	56.5250	0.11271	0.11286	57.5539	7.208	7.217	0.2151
55.7726	56.6836	0.11264	0.11283	57.9319	7.207	7.210	0.2603

Table 2. (Continued)

$\vartheta_0/^\circ\text{C}$	$\vartheta_\lambda/^\circ\text{C}$	$\lambda/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\lambda_c/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\vartheta_a/^\circ\text{C}$	$a^a/10^{-8}\text{m}^2\cdot\text{s}^{-1}$	$a_c^a/10^{-8}\text{m}^2\cdot\text{s}^{-1}$	$(Q_0/4\pi\lambda)/\text{K}$
1,2,3-Trimethylbenzene (Hemimellitene) Data (Measured with Cell AC)							
21.8707	22.4317	0.12807	0.12795	23.2815	8.040	8.013	0.1302
21.8709	22.6620	0.12794	0.12791	23.8565	8.010	8.005	0.1845
21.8709	22.8361	0.12791	0.12788	24.3019	8.041	7.999	0.2232
2.6787	3.2058	0.13121	0.13118	3.9997	8.246	8.279	0.1233
2.6790	3.4277	0.13119	0.13114	4.5593	8.212	8.271	0.1746
2.6791	3.5828	0.13114	0.13112	4.9478	8.197	8.266	0.2112
-16.0577	-15.5301	0.13415	0.13433	-14.6995	8.597	8.537	0.1166
-16.0576	-15.3158	0.13399	0.13430	-14.1533	8.552	8.529	0.1651
-16.0578	-15.1577	0.13398	0.13427	-13.7451	8.557	8.524	0.2000
9.6618	10.2005	0.13034	0.13001	11.0168	8.155	8.182	0.1255
9.6620	10.4244	0.13021	0.12997	11.5785	8.139	8.174	0.1779
9.6617	10.5877	0.13018	0.12994	11.9934	8.150	8.168	0.2153
39.0703	39.6444	0.12521	0.12506	40.4996	7.791	7.775	0.1362
39.0707	39.8891	0.12515	0.12502	41.1127	7.808	7.767	0.1931
39.0709	40.0567	0.12506	0.12499	41.5256	7.780	7.761	0.2339
57.0046	57.5884	0.12185	0.12204	58.4387	7.488	7.528	0.1429
57.0045	57.8446	0.12179	0.12200	59.0787	7.534	7.519	0.2026
57.0046	58.0166	0.12170	0.12197	59.4989	7.510	7.513	0.2454
1,2,4-Trimethylbenzene (Pseudocumene) Data (Measured with Cell BD)							
21.8708	22.3859	0.12774	0.12751	23.1455	8.262	8.280	0.1283
21.8703	22.6058	0.12766	0.12747	23.6947	8.283	8.271	0.1818
21.8708	22.7563	0.12751	0.12744	24.0644	8.255	8.264	0.2200
2.6788	3.1815	0.13140	0.13120	3.9393	8.609	8.604	0.1211
2.6789	3.3890	0.13126	0.13116	4.4578	8.583	8.595	0.1717
2.6783	3.5414	0.13120	0.13113	4.8440	8.597	8.588	0.2077
-16.0569	-15.5715	0.13452	0.13481	-14.8279	8.886	8.920	0.1144
-16.0565	-15.3636	0.13440	0.13477	-14.2966	8.911	8.911	0.1619
-16.0565	-15.2158	0.13441	0.13474	-13.9193	8.919	8.905	0.1960
9.6616	10.1676	0.13013	0.12986	10.9233	8.478	8.486	0.1236
9.6621	10.3883	0.13002	0.12982	11.4808	8.515	8.476	0.1753
9.6609	10.5309	0.12994	0.12979	11.8330	8.471	8.470	0.2121
39.0719	39.6039	0.12435	0.12420	40.3782	7.999	7.989	0.1348
39.0717	39.8283	0.12420	0.12415	40.9316	8.000	7.980	0.1911
39.0707	39.9781	0.12412	0.12413	41.2945	7.956	7.974	0.2317
57.0044	57.5450	0.12051	0.12075	58.3147	7.650	7.687	0.1421
57.0045	57.7813	0.12048	0.12070	58.8945	7.692	7.677	0.2013
57.0049	57.9429	0.12041	0.12067	59.2849	7.676	7.670	0.2440
1,3,5-Trimethylbenzene (Mesitylene) Data (Measured with Cell BD)							
22.8086	23.2110	0.13576	0.13544	23.7785	8.995	9.024	0.1212
22.8085	23.3844	0.13564	0.13540	24.1990	9.015	9.015	0.1719
22.8091	23.5090	0.13558	0.13537	24.5005	9.020	9.009	0.2082
-14.8802	-14.4890	0.14344	0.14372	-13.9165	9.774	9.834	0.1078
-14.8797	-14.3154	0.14341	0.14368	-13.4836	9.834	9.825	0.1528
-14.8797	-14.1967	0.14332	0.14366	-13.1901	9.823	9.818	0.1851
3.3226	3.7288	0.13998	0.13972	4.3169	9.485	9.442	0.1141
3.3230	3.8933	0.13982	0.13968	4.7167	9.438	9.434	0.1620
3.3225	4.0140	0.13982	0.13966	5.0137	9.446	9.427	0.1958
39.8752	40.2925	0.13194	0.13169	40.8758	8.711	8.657	0.1277
39.8753	40.4542	0.13168	0.13165	41.2590	8.627	8.649	0.1813
39.8759	40.5769	0.13167	0.13162	41.5521	8.629	8.642	0.2194
58.4223	58.8397	0.12741	0.12761	59.4126	8.277	8.259	0.1351
58.4234	59.0097	0.12736	0.12757	59.8130	8.248	8.250	0.1916
58.4237	59.1255	0.12718	0.12755	60.0853	8.207	8.244	0.2321

<sup>a</sup> Thermal diffusivity values were adjusted by a factor of  $k_f$ .

of such isomers are naturally close to those (especially close in heat capacity) of the sample. Therefore, given the additivity rules for thermal properties of a mixture, the impurities (isomers; 1% to 2% contents) might not severely affect the results beyond the estimated uncertainty for the measurement (also, cf. the comment on 1,4-cyclohexadiene in the Evaluation of Uncertainty).

**Experimental Data.** The experiments with the 29 materials (liquids) were carried out at three heating rates  $Q_0$  at a bath temperature  $\vartheta_0/^\circ\text{C}$  ( $T_0/\text{K} - 273.15$ ) for respective cell settings. The measured data  $\lambda$  and  $a$  are summarized in Table 2 together with the values  $\lambda_c$  and  $a_c$  calculated by the fitting formulas

$$\lambda/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1} = \lambda_0/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1} - A(\vartheta/^\circ\text{C}) \quad (1)$$

and

$$a/10^{-8}\text{m}^2\cdot\text{s}^{-1} = a_0/10^{-8}\text{m}^2\cdot\text{s}^{-1} - B(\vartheta/^\circ\text{C}) \quad (2)$$

which are derived from the pair of data ( $\lambda$  and  $\vartheta_\lambda$ ) and ( $a$

and  $\vartheta_a$ ) in Table 2, respectively, where  $\vartheta_\lambda/^\circ\text{C}$  ( $T_\lambda/\text{K} - 273.15$ ) and  $\vartheta_a/^\circ\text{C}$  ( $T_a/\text{K} - 273.15$ ) are the effective temperatures referred to for measured  $\lambda$  and  $a$ , while these data are the mean of two results (sets A and C data with cell AC or sets B and D data with cell BD) obtained experimentally with an equivalent heating rate of  $Q_0$  to reduce the amount of data. The heating parameter  $Q_0/4\pi\lambda$  represents an index of heating condition in the experiment. The values of the coefficients  $A$  and  $B$  of eqs 1 and 2 are shown in Table 3, where the numbers in parentheses following the coefficients are the numerical values of the standard uncertainties referred to in the corresponding last digits of the quoted results for the intercept and slope.

Figures 1–6 show the deviations for the measured values of the 29 liquids from eqs 1 and 2. It should be pointed out, by looking at these figures, that the result of the thermal conductivity of benzene is very close to the IUPAC-recommended values<sup>8</sup> as shown in Figure 3a.

A comment must be made on the measurement of 1,3-cyclohexadiene. A curious phenomenon was found among the thermal diffusivity data. Figure 7 shows both the data



Table 3. Coefficients of Equations 1 and 2

material	formula	cell	<i>N</i> (data)	$\lambda_0^a/W \cdot m^{-1} \cdot K^{-1}$	$A^a/10^{-4}$	$a_0^a/10^{-8} m^2 \cdot s^{-1}$	$B^a/10^{-2}$
1-pentene	C <sub>5</sub> H <sub>10</sub>	AC	24	0.12227(5)	-3.936(25)	8.865(08)	-2.934(39)
1-hexene	C <sub>6</sub> H <sub>12</sub>	AC	36	0.12582(6)	-3.399(18)	8.829(11)	-2.492(33)
2,3-dimethyl-1-butene	C <sub>6</sub> H <sub>12</sub>	BD	36	0.11241(5)	-3.052(14)	7.861(13)	-2.346(34)
2,3-dimethyl-2-butene	C <sub>6</sub> H <sub>12</sub>	AC	36	0.13035(5)	-3.563(13)	9.067(14)	-2.734(39)
1-heptene	C <sub>7</sub> H <sub>14</sub>	AC	24	0.12913(5)	-3.131(19)	8.890(09)	-2.302(30)
1-octene	C <sub>8</sub> H <sub>16</sub>	AC	30	0.13129(5)	-2.966(15)	8.695(18)	-2.584(55)
cyclopentene	C <sub>5</sub> H <sub>8</sub>	AC	24	0.14260(6)	-4.324(24)	10.706(09)	-4.003(35)
cyclohexene	C <sub>6</sub> H <sub>10</sub>	AC	36	0.13539(5)	-3.208(15)	9.637(14)	-3.066(42)
cyclopentane	C <sub>5</sub> H <sub>10</sub>	BD	30	0.13623(4)	-3.945(15)	10.502(13)	-4.176(52)
cyclohexane	C <sub>6</sub> H <sub>12</sub>	BD	24	0.12531(7)	-2.858(23)	8.989(15)	-3.077(51)
cyclohexane- <i>d</i> <sub>12</sub>	C <sub>6</sub> D <sub>12</sub>	BD	30	0.11809(5)	-2.654(14)	6.994(14)	-2.399(39)
methylcyclopentane	C <sub>6</sub> H <sub>12</sub>	BD	24	0.12250(3)	-3.183(14)	8.971(09)	-3.050(38)
cycloheptane	C <sub>7</sub> H <sub>14</sub>	BD	24	0.12449(3)	-2.431(10)	8.613(10)	-2.454(38)
cyclooctane	C <sub>8</sub> H <sub>16</sub>	AC	26	0.12377(6)	-2.136(16)	7.799(11)	-1.866(29)
benzene	C <sub>6</sub> H <sub>6</sub>	AC	24	0.14895(3)	-3.255(11)	9.956(14)	-2.098(45)
benzene- <i>d</i> <sub>6</sub>	C <sub>6</sub> D <sub>6</sub>	AC	30	0.14223(5)	-3.192(15)	8.332(11)	-1.949(30)
1,3-cyclohexadiene	C <sub>6</sub> H <sub>8</sub>	AC	36	0.14016(6)	-3.057(19)	9.567 <sup>b</sup>	-2.445 <sup>b</sup>
1,4-cyclohexadiene	C <sub>6</sub> H <sub>8</sub>	BD	36	0.15344(3)	-3.481(09)	10.164(06)	-2.802(20)
toluene- <i>d</i> <sub>8</sub>	C <sub>7</sub> D <sub>8</sub>	BD	30	0.13135(3)	-2.656(09)	8.069(08)	-2.126(24)
bicyclo[2.2.1]hepta-2,5-diene	C <sub>7</sub> H <sub>8</sub>	AC	30	0.14401(7)	-3.132(22)	10.321(13)	-3.554(36)
ethylbenzene	C <sub>8</sub> H <sub>10</sub>	AC	30	0.13375(4)	-2.491(12)	9.167(05)	-2.072(15)
1,2-dimethylbenzene	C <sub>8</sub> H <sub>10</sub>	BD	30	0.13396(7)	-2.091(20)	8.900(14)	-1.883(42)
1,3-dimethylbenzene	C <sub>8</sub> H <sub>10</sub>	AC	36	0.13567(4)	-2.497(12)	9.517(06)	-2.199(20)
1,4-dimethylbenzene	C <sub>8</sub> H <sub>10</sub>	BD	24	0.13314(4)	-2.540(10)	9.277(16)	-2.210(43)
<i>n</i> -propylbenzene	C <sub>9</sub> H <sub>12</sub>	AC	30	0.13320(3)	-2.188(10)	8.895(09)	-1.845(27)
(1-methylethyl)-benzene	C <sub>9</sub> H <sub>12</sub>	BD	30	0.12408(4)	-1.985(13)	8.259(07)	-1.810(20)
1,2,3-trimethylbenzene	C <sub>9</sub> H <sub>12</sub>	AC	36	0.13172(6)	-1.681(18)	8.334(10)	-1.380(31)
1,2,4-trimethylbenzene	C <sub>9</sub> H <sub>12</sub>	BD	36	0.13181(5)	-1.923(17)	8.670(07)	-1.686(22)
1,3,5-trimethylbenzene	C <sub>9</sub> H <sub>12</sub>	BD	36	0.14054(5)	-2.197(21)	9.535(10)	-2.148(29)

<sup>a</sup> The numbers in parentheses following the coefficients are the numerical values of the standard uncertainties referred to in the corresponding last digits. Results were derived from data obtained with the cell AC and BD. <sup>b</sup> Fitted using the measured values at the three higher temperatures.

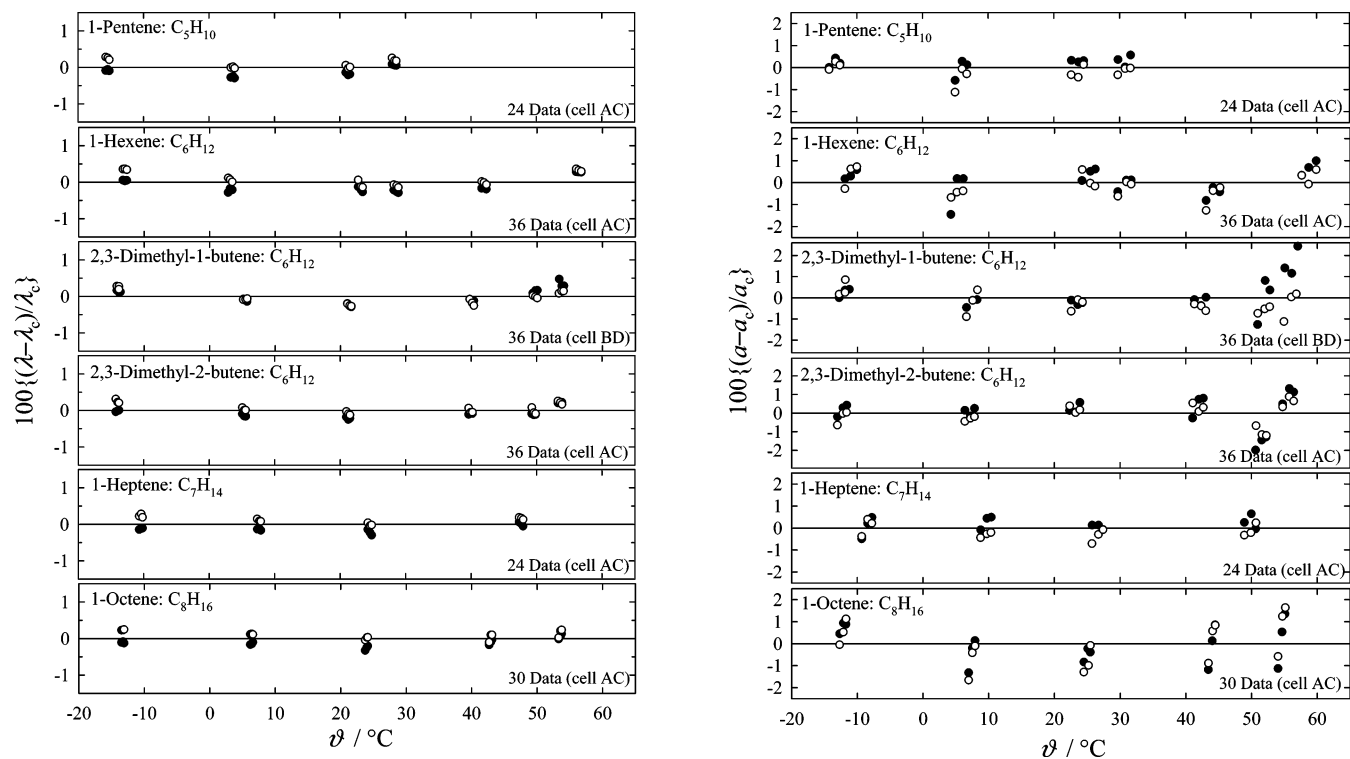
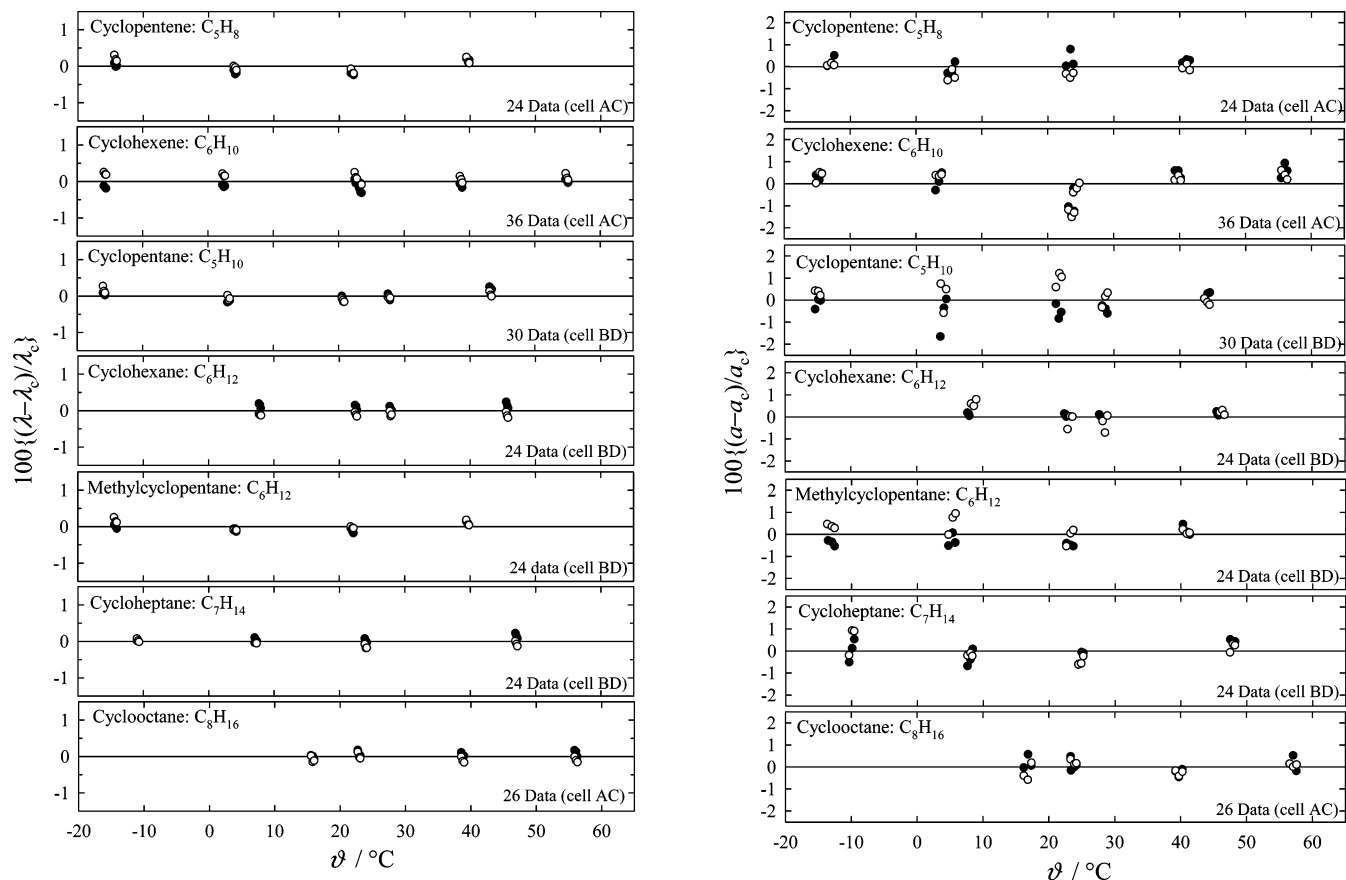


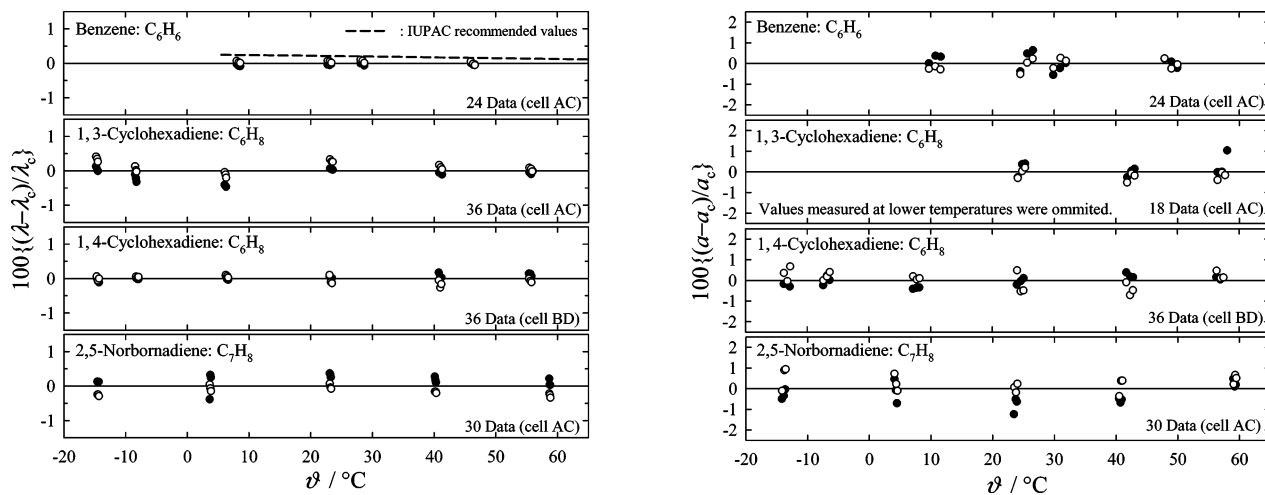
Figure 1. Deviations of measured values from the formulas respectively fitted for six alkenes  $C_nH_{2n}$  ( $n = 5-8$ ) (a) thermal conductivity and (b) thermal diffusivity. Values were adjusted by a factor of  $k_f$ .

of 1,3- and 1,4-cyclohexadienes, where the data were obtained in due sequence of  $\vartheta_0 = 22.53$  °C, 40.20 °C, 54.75 °C, 5.73 °C, -8.78 °C, and -15.16 °C, respectively, under nearly the same times and conditions. The thermal diffusivities of 1,3-cyclohexadiene at the three higher temperatures indicate ordinary behavior as in those of 1,4-cyclohexadiene but showed a clear peculiarity at the three lower temperatures. On the other hand, the thermal conductivities do not seem to clearly indicate the anomaly

in Figure 7, though the difference between the temperature dependences at the lower and higher temperatures is observed, if examining minutely, as far as seen in Figure 3a. The heat capacity at 298.15 K of 1,3-cyclohexadiene derived from  $\lambda$  and  $a$  at the three higher temperatures is consistent with the value in the literature (see Table 5). The density values of samples (1,3- and 1,4-cyclohexadiene), which were taken out from cells after the experiments, were measured as mentioned later. Subsequently,



**Figure 2.** Deviations of measured values from the formulas respectively fitted for cyclopentene and -hexene and five cycloalkanes of  $C_nH_{2n}$  ( $n = 5-8$ ) including methylcyclopentane (a) thermal conductivity and (b) thermal diffusivity. Values were adjusted by a factor of  $k_f$ . ●, Set A data with cell AC or set B data with BD cell; ○, set C data with cell AC or set D data with cell BD, respectively.



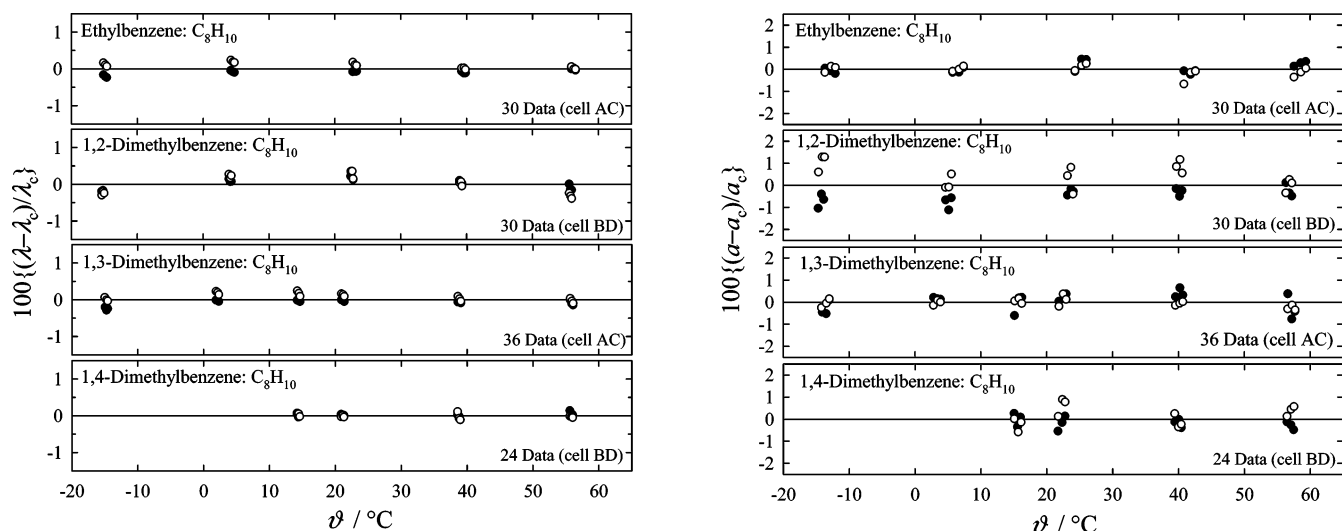
**Figure 3.** Deviations of measured values from the formulas respectively fitted for benzene, 1,3- and 1,4-cyclohexadienes, and norbornadiene: (a) thermal conductivity and (b) thermal diffusivity. Values were adjusted by a factor of  $k_f$ . Fitting values of 1,3-hexadiene were obtained from three higher temperatures. ●, Set A data with cell AC or set B data with the cell BD; ○, set C data with cell AC or set D data with cell BD, respectively.

benzene- $d_6$  with cell AC and cyclohexane- $d_{12}$  with cell BD were measured, and the results were properly conducted. The mode between the cells AC and BD was changed manually with a mercury contact switch, and the abnormal working in the only measurement with the cell AC was not taken into consideration. Therefore the measurement of 1,3-cyclohexadiene is regarded to have been successfully carried out.

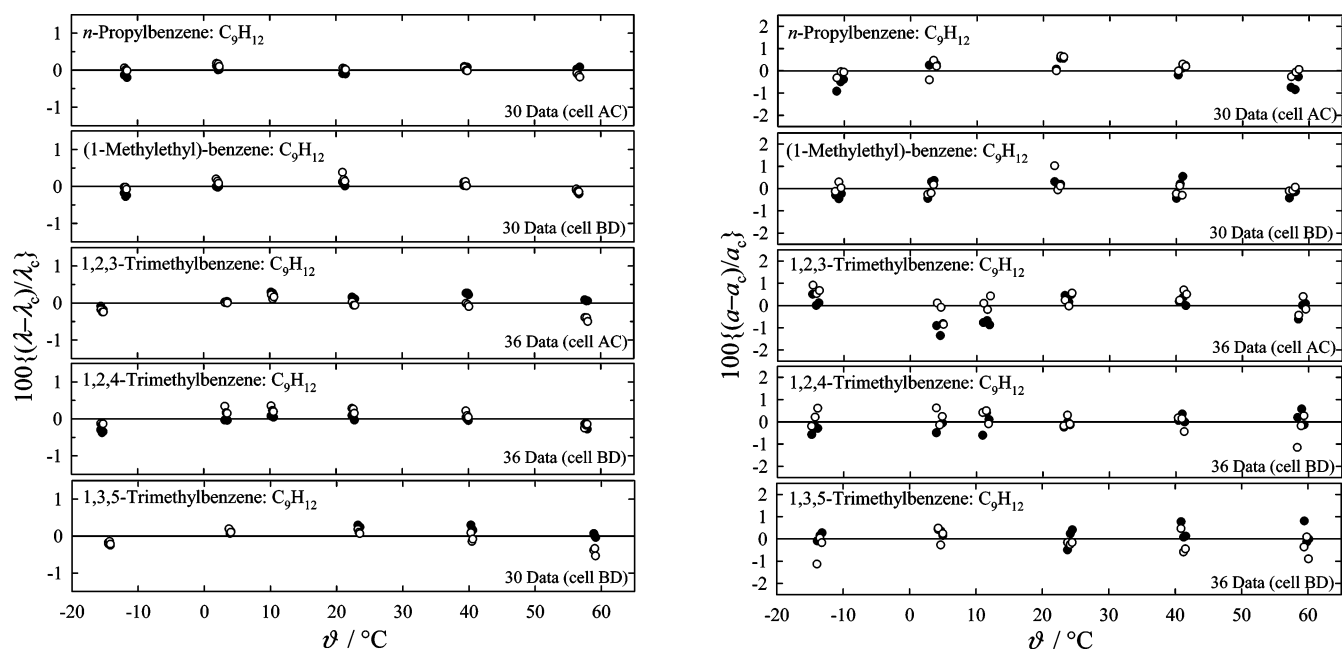
#### **Comparison between Reported and Present Values of Thermal Conductivity.**

A comparison between the

previously reported data in the literature<sup>9-48</sup> and the present results is shown chronologically in Table 4 except for the cases of some materials for which the thermal conductivity was not found. These were not intentionally selected, and their uncertainty is mostly unclear. Therefore, we did not examine each difference between the referred and present data. Additionally, the differences do not arise from the purity of the sample but most naturally from the variance among the individual data obtained by various researchers with their respective techniques.



**Figure 4.** Deviations of measured values from the formulas respectively fitted for ethylbenzene and relatives: (a) thermal conductivity and (b) thermal diffusivity. Values were adjusted by a factor of  $k_f$ . ●, Set A data with cell AC or set B data with the cell BD; ○, set C data with cell AC or set D data with cell BD, respectively.



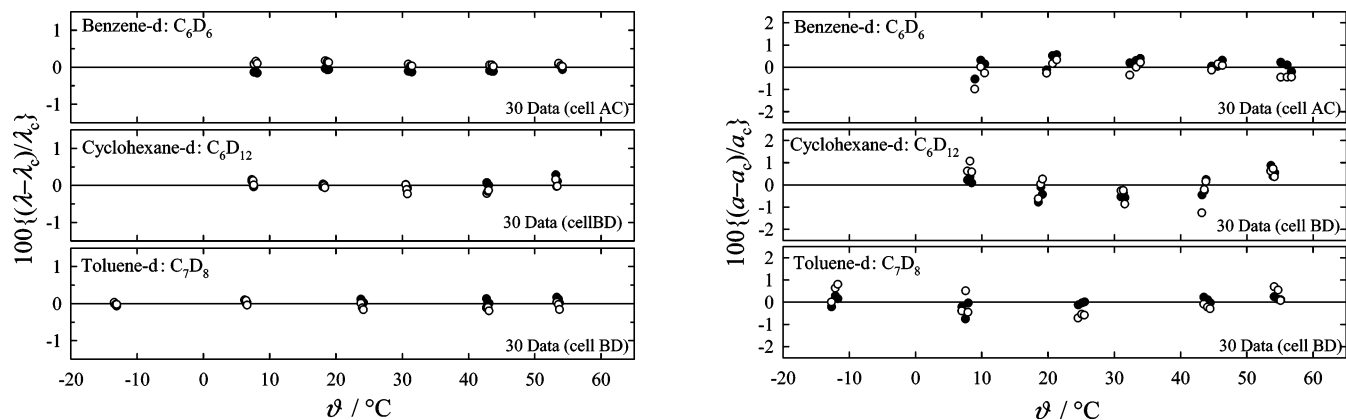
**Figure 5.** Deviations of measured values from the formulas respectively fitted for propylbenzene and relatives: (a) thermal conductivity and (b) thermal diffusivity. Values were adjusted by a factor of  $k_f$ . ●, Set A data with cell AC or set B data with the cell BD; ○, set C data with cell AC or set D data with cell BD, respectively.

Some of the values are calculated from the formula as smoothed values, and the present results (in parentheses) are calculated at the same temperatures reported using eq 1 with the coefficients listed in Table 3.

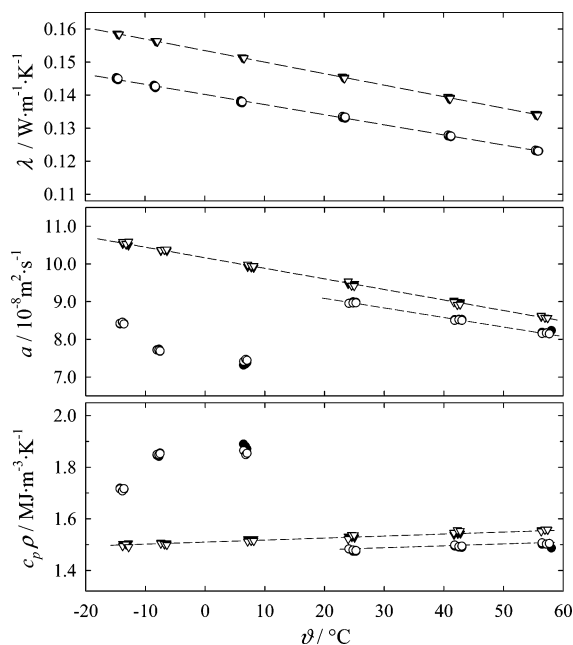
**Summarized Results at 298.15 K.** Table 5 lists the values determined for the properties at a nominal temperature of 298.15 K together with the values of the molar heat capacity (with a previously obtained result of toluene).<sup>2</sup> The massic heat capacity at constant pressure  $c_p$  can be derived from the thermal conductivity  $\lambda$ , the thermal diffusivity  $a$ , and the density  $\rho$  using the equation  $a = \lambda / c_p \rho$ . The densities of the sample were conventionally obtained from the literature,<sup>7</sup> together with molar mass, but since those of six materials (cyclohexane- $d_{12}$ , benzene- $d_6$ , 1,3- and 1,4-cyclohexadienes, toluene- $d_8$  and norbornadiene) are unavailable, they were measured using a vibrating tube densimeter (Anton Parr DMA5000 SH3). The density values in the literature are believed to be sufficient by

experience for the purpose of deriving the heat capacity. The various (volumic,  $c_{p\rho}$ ; massic,  $c_p$ ; molar,  $C_{m,p}$ ) heat capacities are in agreement with most of the values  $C_{m,p}$  found in the literatures, although the reliability of the values were not perfectly examined.<sup>6,7,49–58</sup> As exceptions, the values of some materials (for example, norbornadiene, 1,3-dimethylbenzene, 1-heptene, and an especially large value for norbornadiene) differed by more than 1.8% (i.e., estimated uncertainty) from those referred to from the literature. The  $c_{p\rho}$  of norbornadiene (an isomer of toluene), however, is very close to that of toluene, although their thermal conductivity, thermal diffusivity, and density are quite different from each other.

The thermal properties are considered to naturally have relevance to the boiling point, density, and/or molar density. Prediction of thermal properties of pure organic liquids has been specially investigated, relating to the molar density.<sup>59,60</sup> Therefore the consistency of the mea-



**Figure 6.** Deviations of measured values from the formulas respectively fitted for three deuterated hydrocarbons: (a) thermal conductivity and (b) thermal diffusivity. Values were adjusted by a factor of  $k_f$ . ●, Set A data with cell AC or set B data with the cell BD; ○, set C data with cell AC or set D data with cell BD, respectively.



**Figure 7.** Values of 1,3-cyclohexadiene measured with cell AC and 1,4-cyclohexadienes with cell BD. The volumic heat capacity  $c_p\rho$  is calculated by  $\lambda_c/a_m$  ( $\lambda_c$ , calculated from the fitting equation;  $a_m$ , measured value) referred to the temperature  $\vartheta_a$ . Measurements were made in due sequence of  $\vartheta_0 = 22.53$  °C, 40.20 °C, 54.75 °C, 5.73 °C, -8.78 °C, and -15.16 °C at the same time and under the same condition for both materials. ●, Set A data of 1,3-cyclohexadiene; ○, set C data of 1,3-cyclohexadiene; ▼ set B data of 1,4-cyclohexadiene; ▽ set D data of 1,4-cyclohexadiene.

surement of thermal conductivity and thermal diffusivity was examined by comparing the molar heat capacities representatively. Figure 8 shows the molar heat capacities,  $C_{m,p} = (\lambda/a)(M/\rho)$ , of 29 materials together with some of the alkanes and the toluene previously obtained.<sup>2,3</sup> As mentioned above, the heat capacity  $C_{m,p}$  of norbornadiene differs greatly (9.2%) from the referred value, but that value was only found in the literature.<sup>57</sup> Figure 8 shows that the values of  $C_{m,p}$  of both toluene (g1) and norbornadiene (g2,  $C_7H_8$ ) are arranged according to the values  $\rho/M$  with a proper tendency, excluding the deuterated materials. Judging from this situation, the present molar heat capacity of norbornadiene might be more reliable than the referred one.

Furthermore it is interesting that norbornadiene and 1,4-cyclohexadiene show almost the same  $a$  value (although  $\lambda$ ,  $c_p$ ,  $c_p\rho$ , and  $C_{m,p}$  differ from each other), because both their

structures are  $C_6$  cyclic rings, their boiling points are almost the same, and they have double bonds on each opposite side of ring.

**Thermal Properties of Deuterated Liquids.** The thermal properties of three deuterated liquids (benzene- $d_6$ , toluene- $d_8$ , and cyclohexane- $d_{12}$ ) were compared with those of their ordinary hydrocarbons ( $\lambda$  of toluene).<sup>2</sup> Horrocks et al. presented a relationship of the ratio  $\lambda_H/\lambda_D$  of both deuterated and ordinary hydrocarbons to the ratio  $M_D/M_H$  as follows<sup>20</sup>

$$\lambda_H/\lambda_D \approx (M_D/M_H)^{1/2} \quad (3)$$

where  $M_D$  and  $M_H$  are the molar masses of the deuterated and ordinary materials. Table 6 shows the relative values,  $\lambda_H/\lambda_D$ ,  $a_H/a_D$ , and  $(C_{m,p})_H/(C_{m,p})_D$ , which are calculated from Table 5, together with  $\lambda_H/\lambda_D$  for  $C_6H_6/C_6D_6$  ( $\lambda_H = 0.1426$  at 295.85 K and  $\lambda_D = 0.1373$  at 295.95 K) and  $C_6H_{12}/C_6D_{12}$  ( $\lambda_H = 0.1201$  at 294.55 K and  $\lambda_D = 0.1133$  at 295.35 K) reported by Horrocks et al.<sup>20</sup> The present results of  $\lambda_H/\lambda_D$  are consistent by around 1% with the relationship (eq 3) and with those of Horrocks et al. Furthermore, it is very interesting that values  $a_H/a_D$  and  $(C_{m,p})_H/(C_{m,p})_D$  of the two aromatics (benzene and toluene) are very close to those of the other material, although those of cyclohexane are observed to be clearly different from benzene and toluene.

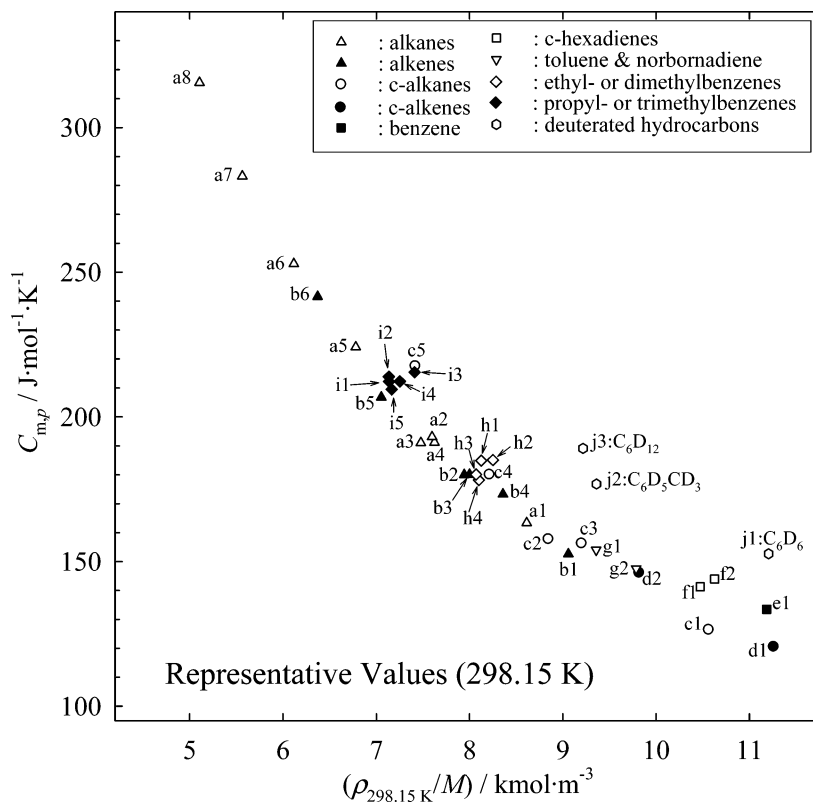
**Evaluations of Uncertainty.** The evaluation of the uncertainty components in the measurement was made using the simplified working formula

$$\Delta T = (Q_0/4\pi\lambda) \ln(t/s) + (Q_0/4\pi\lambda) \ln(4as/r^2C) \quad (4)$$

The uncertainty in the thermal conductivity can be evaluated as<sup>3,4</sup>

$$\frac{\delta\lambda}{\lambda} = \frac{\delta Q_0}{Q_0} + \frac{\delta(dR_W/dT)}{dR_W/dT} + \frac{\delta(\Delta T_f - \Delta T_i)}{\Delta T_f - \Delta T_i} + \frac{\delta\tau(t_f - t_i)}{t_f \ln(t_f/t_i)} + \left(\frac{\delta\lambda}{\lambda}\right)_{\text{sample}} + \left(\frac{\delta\lambda}{\lambda}\right)_{\text{pressure}} + \left(\frac{\delta\lambda}{\lambda}\right)_{\text{others}} \quad (5)$$

where  $\delta(*)$  is the uncertainty of the (\*) terms,  $R_W$  the resistance of the hot-wire sensor, and  $\delta\tau$  the ambiguity of the time lag of both trigger signals to the bridge and the digital voltmeter. The magnitude of the respective components, contributing as a random or systematic part, is the same as that in the previous study.<sup>4</sup> The first component is 0.17%, in terms of the standard uncertainty (as a random part, type A), the second is ~0.05% (as a systematic part, type A), the third is ~0.05% (as a random part, type A),



**Figure 8.** Molar heat capacities calculated at 298.15 K vs molar density together with those of some alkanes.<sup>2,3</sup> Materials and symbols are designated as follows: a1, pentane; a2, hexane; a3, 2,2-dimethylbutane; a4, 2,3-dimethylbutane; a5, heptane; a6, octane; a7, nonane; a8, decane; b1, 1-pentene; b2, 1-hexene; b3, 2,3-dimethyl-1-butene; b4, 2,3-dimethyl-2-butene; b5, 1-heptene; b6, 1-octene; c1, cyclopentane; c2, methylcyclopentane; c3, cyclohexane; c4, cycloheptane; c5, cyclooctane; d1, cyclohexene; d2, cyclohexane; e1, benzene; f1, 1,3-cyclohexadiene; f2, 1,4-cyclohexadiene; g1, toluene; g2, bicyclo[2.2.1]hepta-2,5-diene (norbornadiene); h1, ethylbenzene; h2, 1,2-dimethylbenzene (*o*-xylene); h3, 1,3-dimethylbenzene (*m*-xylene); h4, 1,4-dimethylbenzene (*p*-xylene); i1, *n*-propylbenzene; i2, (1-methylethyl)benzene (isopropylbenzene); i3, 1,2,3-trimethylbenzene (hemimellitene); i4, 1,2,4-trimethylbenzene (pseudocumene); i5, 1,3,5-trimethylbenzene (mesitylene); j1, benzene-*d*<sub>6</sub>; j2, toluene-*d*<sub>6</sub>; j3, cyclohexane-*d*<sub>12</sub>.

and the fourth is negligible. The fifth (the sample material) is rather difficult to estimate because of the lack of exact information concerning purity. However, most of the impurities are thought to be isomers (as mentioned before) and are expected to be less than 2% (although hemimellitene certainly contains extra impurities (this means other isomers)). Since the sample of 1,4-cyclohexadiene contains ~3% benzene, the corrections were made to values of 100% substances of 1,4-cyclohexadiene using the results of benzene and the magnitudes were 0.08% for  $\lambda$ , 0.01% for  $a$ , and 0.07% for  $c_{p\rho}$ , respectively. Therefore, this fifth term is assumed to be ~0.10% (as a random part, type B) and the other components, including the potential lead, and the sampling time-step distribution, etc., ~0.04% (a random part, mixed types A and B). Overall, the combined standard uncertainty is about 0.24%, evaluated as the root-sum square of the various components.

For measurement of the thermal diffusivity, the original uncertainty ( $2\delta r/r$ ) is replaced by the term  $(\delta a/a)_{\text{cal}} = (\delta k_f/k_f)$  since the adjustment of the diameter of the wire has been made for respective configurations, and the uncertainty is evaluated as follows<sup>3,4</sup>

$$\delta a/a = (\delta a/a)_{\text{cal}} + \delta(\Delta T)_0/(Q_0/4\pi\lambda) + (\delta\lambda/\lambda)^* \ln(4as/r^2C) + (\delta a/a)_{\text{sample}} \quad (6)$$

In this formula, the first term cannot be evaluated precisely but can tentatively be said to be 0.3% (a systematic part, type B), and the second term  $\delta(\Delta T)_0$ , the initially remaining deflection in terms of temperature, originating from an

inadequate balance in the bridge at temperature  $T_0$  is about 0.5% (a random part, type B). According to the third term, subcomponents  $\delta Q_0/Q_0$  and  $(\delta\lambda/\lambda)_{\text{material}}$  in eq 6 do not practically affect  $\delta a/a$ , and therefore,  $(\delta\lambda/\lambda)^*$  is 0.084%. This term is estimated to be 0.67% ( $\ln(4as/r^2C) \approx 8$ ) (a random part, type A). The last term  $(\delta a/a)_{\text{sample}}$  is actually the same as  $(\delta\lambda/\lambda)_{\text{material}}$  and is 0.10% (a random part, type B). Finally, the overall uncertainty is estimated to be 0.90%, computed as the root-sum-square of the subcomponents.

## Discussion and Conclusions

The original data on the thermal conductivity and thermal diffusivity for the 29 materials of alkenes, cycloalkanes, cycloalkanes, benzene and its relatives, and deuterated hydrocarbons are reported. The various heat capacities were derived at the nominal temperature of 298.15 K from the ratio of the thermal conductivity to the thermal diffusivity  $\lambda/\kappa$ , the density  $\rho$ , and the molar mass  $M$ ,<sup>7</sup> where a part of the density values were measured using a vibrating tube densimeter. The derived  $c_p$  (or  $C_{m,p}$ ) seems consistent enough with the values from the literature within the estimated uncertainty of the experimental system (excluding some materials: 1-heptene, norbornadiene, and 1,3-dimethylbenzene), although all of referred values may be not reliable with a high level. The volumic heat capacity of norbornadiene  $c_{p\rho} = \lambda/a$  is very close to that of toluene, which is an isomer, although  $\lambda$ ,  $a$ , and  $\rho$  differ from each other. The consistency of the measurement of thermal conductivity and thermal diffusivity was examined and confirmed by comparing the molar heat capacities representatively. The deuterated hydrocarbons behave

**Table 4. Examples of Literature Values of Thermal Conductivity under 1013.25 hPa or Saturation Pressure Together with Present Data (in Parentheses) Calculated at the Same Temperature from Equation 1 with the Coefficients Listed in Table 3**

material	literature value	year	method <sup>a</sup>	source	
1-hexene	0.1249(0.12417: 4.86 °C), 0.1177(0.11619: 28.32 °C), 0.1119(0.11049: 45.10 °C)	1968	SHW	9	
	0.1130(0.11659: 27.15 °C), 0.1047(0.10874: 50.25 °C)	1990	THW	10	
1-heptene	0.1277(0.12741: 5.50 °C), 0.1189(0.11769: 36.54 °C), 0.1174(0.11661: 40.00 °C)	1968	SHW	9	
	0.1224(0.12284: 20.09 °C), 0.1172(0.11719: 38.12 °C), 0.1115(0.11077: 58.64 °C)	1988	THW	11	
	0.12599(0.12287: 20 °C)	1992	THW	12	
1-octene	0.1271(0.11943: 40 °C), 0.1184(0.11349: 60 °C)	1955	PP	13	
	0.1303(0.12959: 5.74 °C), 0.1248(0.12367: 25.70 °C), 0.1157(0.11346: 60.10 °C)	1968	SHW	9	
	0.1212(0.12106: 34.5 °C), 0.1185(0.11720: 47.5 °C)	1987	THW	14	
	0.1257(0.12393: 24.81 °C), 0.1252(0.12307: 27.72 °C)	1988	THW	11	
	0.1111(0.11606: 51.35 °C)	1990	THW	10	
cyclopentene	0.1500(0.14260: 0 °C), 0.1435(0.13180: 25 °C)	1983	SHW	15	
	0.1341(0.12737: 25 °C)	1957	PP	16	
cyclohexene	0.1286(0.12733: 25.13 °C), 0.1231(0.12295: 38.77 °C), 0.1172(0.11603: 60.36 °C)	1981	CC	17	
	0.1421(0.13539: 0 °C), 0.1342(0.11935: 50 °C)	1983	SHW	15	
	0.1322(0.13180: 25 °C)	1957	PP	16	
cyclopentane	0.1267(0.12719: 22.91 °C), 0.1200(0.12031: 40.36 °C)	1981	CC	17	
	0.1439(0.13623: 0 °C), 0.1315(0.12637: 25 °C)	1983	SHW	15	
	0.1406(0.14042: -10.629 °C), 0.1290(0.12830: 20.096 °C), 0.1238(0.12237: 35.138 °C)	2001	THW	18	
methylcyclopentane	0.1192(0.11454: 25 °C)	1957	PP	16	
	0.1295(0.12250: 0 °C), 0.1179(0.10659: 50 °C)	1983	SHW	15	
	0.1228(0.11817: 25 °C)	1957	PP	16	
cyclohexane	0.1239(0.11959: 20 °C)	1957	CC	19	
	0.1201(0.11919: 21.4 °C), 0.1187(0.11645: 31.0 °C), 0.1107(0.10839: 59.2 °C)	1963	THW	20	
	0.124(0.11959: 20 °C)	1979	ACHR	21	
	0.1177(0.11809: 25.27 °C), 0.1153(0.11378: 40.36 °C), 0.1103(0.11115: 49.55 °C)	1981	CC	17	
	0.1201(0.11674: 30 °C)	1982	RTHW	22	
	0.1176(0.11817: 25 °C), 0.1119(0.11102: 50 °C)	1984	SHW	23	
	0.1148(0.11502: 36.0 °C), 0.1159(0.11073: 51.0 °C)	1984	THW	24	
	0.1144(0.11388: 40 °C)	1988	THW	25	
	0.1178(0.12245: 10 °C), 0.1140(0.11817: 25 °C), 0.1080(0.11102: 50 °C)	1988	THW	26	
	0.1083 (at 0.3MPa)(0.11006: 53.35 °C)	1989	THW	27	
	0.1133(0.11220: 22.2 °C), 0.1113(0.10986: 31.0 °C), 0.1040(0.10193: 60.9 °C)	1963	THW	20	
	0.1262(0.12449: 0 °C), 0.1213(0.11841: 25 °C), 0.1169(0.11234: 50 °C)	1983	SHW	15	
	0.1203(0.11843: 25 °C), 0.1172(0.11309: 50 °C)	1983	SHW	15	
	0.1453(0.14244: 20 °C)	1957	CC	19	
	cyclohexane- <i>d</i> <sub>12</sub>	0.1426(0.14156: 22.7 °C), 0.1387(0.13759: 34.9 °C), 0.1316(0.12963: 59.35 °C)	1963	THW	20
0.1430(0.14081: 25 °C)		1966	CC	28	
0.1424(0.14081: 25 °C)		1967	PP	29	
0.146(0.14244: 20 °C), 0.139(0.13593: 40 °C), 0.133(0.12942: 60 °C)		1978	THW	30	
0.1511(0.14244: 20 °C), 0.1461(0.13593: 40 °C), 0.1432(0.13268: 50 °C)		1980	PP	31	
0.149(0.14244: 20 °C)		1981	ACHW	32	
0.1372(0.13919: 30 °C)		1982	RTHW	22	
0.1433(0.14081: 25 °C), 0.1376(0.13268: 50 °C)		1984	SHW	23	
0.1366(0.13690: 37.0 °C), 0.1335(0.13349: 47.5 °C)		1984	THW	24	
0.1495(0.14081: 25 °C), 0.1457(0.13593: 40 °C)		1985	PP	33	
0.1358(0.13593: 40 °C)		1988	THW	25	
0.1419(0.14067: 25.43 °C), 0.1379(0.13696: 36.85 °C), 0.1300(0.12936: 60.17 °C)		1988	THW	34	
0.1455(0.14570: 10 °C), 0.1397(0.14081: 25 °C), 0.1304(0.13268: 50 °C)		1988	THW	26	
0.14012(0.14064: 25.53 °C), 0.13706(0.13710: 36.40 °C), 0.13068(0.13000: 58.22 °C)		1989	THW	35	
0.1429(0.14242: 20.05 °C)		2002	THW	36	
benzene- <i>d</i> <sub>6</sub>	0.1373(0.13498: 22.8 °C), 0.1338(0.13144: 33.8 °C), 0.1267(0.12423: 56.4 °C)	1963	THW	20	
	0.1303(0.12628: 30 °C)	1960	PP&CC	37	
	0.1352(0.13240: 5.42 °C), 0.1339(0.13349: 10.62 °C), 0.1292(0.12500: 35.12 °C)	1968	SHW	9	
	0.1265(0.12550: 33.1 °C), 0.1229(0.12249: 45.2 °C), 0.1203(0.11958: 56.9 °C)	1977	TCC	38	
	0.134(0.12877: 20 °C), 0.128(0.12379: 40 °C), 0.124(0.11880: 60 °C)	1978	THW	30	
	0.1291(0.12752: 25 °C)	1982	RTHW	22	
	0.1306(0.12590: 31.5 °C), 0.1255(0.12229: 46.0 °C)	1986	THW	39	
	0.1286(0.12979: 19.95 °C)	2002	THW	36	
	<i>o</i> -xylene	0.136(0.12978: 20 °C)	1951	CC	40
		0.1361(0.12978: 20 °C)	1957	CC	19
		0.1308(0.12769: 30 °C)	1960	PP&CC	37
		0.1360(0.13281: 5.50 °C), 0.1302(0.12739: 31.44 °C), 0.1292(0.12653: 35.52 °C)	1968	SHW	9
		0.1284(0.12704: 33.1 °C), 0.1248(0.12451: 45.2 °C), 0.1222(0.12206: 56.9 °C)	1977	TCC	38
		0.1323(0.12875: 25 °C)	1982	RTHW	22
		0.1366(0.13396: 0 °C), 0.1302(0.12875: 25 °C), 0.1243(0.12392: 48 °C)	1987	CC	41
0.1296(0.12852: 26.0 °C), 0.1268(0.12604: 37.86 °C), 0.1226(0.12237: 55.43 °C)		1988	THW	42	
0.1303(0.12979: 19.94 °C)		2002	THW	36	
0.1404(0.13937: 5.31 °C), 0.1396(0.13874: 8.18 °C), 0.1331(0.13264: 35.98 °C)		1968	SHW	9	
0.1370(0.13615: 20 °C), 0.1325(0.13175: 40 °C), 0.1280(0.12736: 60 °C)		1971	CC	47	
0.1356(0.13068: 20 °C)		1948	CC	43	
0.1310(0.13068: 20 °C)		1957	CC	19	
0.1297(0.12818: 30 °C)		1960	PP&CC	37	
<i>m</i> -xylene		0.1303(0.12943: 25 °C)	1966	CC	28
	0.1311(0.12943: 25 °C)	1967	PP	29	
	0.1278(0.12740: 33.1 °C), 0.1246(0.12438: 45.2 °C), 0.1215(0.12146: 56.9 °C)	1977	TCC	38	
	0.1306(0.12943: 25 °C)	1982	RTHW	22	
	0.13512(0.13567: 0 °C), 0.12805(0.12943: 25 °C)	1986	THW	44	
	0.1294(0.13068: 19.96 °C)	2002	THW	36	
	<i>p</i> -xylene	0.1361(0.12806: 20 °C)	1957	CC	19
		0.1262(0.12473: 33.1 °C), 0.1244(0.12166: 45.2 °C), 0.1201(0.11869: 56.9 °C)	1977	TCC	38
		0.1314(0.12806: 20 °C), 0.1277(0.12298: 40 °C), 0.1239(0.11790: 60 °C)	1980	PP	31
		0.1299(0.12679: 25 °C)	1982	RTHW	22
		0.1272(0.12642: 26.47 °C), 0.1249(0.12418: 35.27 °C), 0.1201(0.11939: 54.12 °C)	1988	THW	42
		0.1278(0.12812: 19.75 °C)	2002	THW	36

Table 4. (Continued)

material	literature value	year	method <sup>a</sup>	source
<i>n</i> -propylbenzene	0.1267(0.13076: 11.15 °C), 0.1262(0.13046: 12.51 °C), 0.1261(0.13013: 14.03 °C)	1968	SHW	9
	0.130(0.13061: 11.85 °C), 0.122(0.12273: 47.85 °C)	1976	CS	45
isopropylbenzene	0.1318(0.12011: 20 °C)	1948	CC	43
	0.12853(0.12408: 0 °C), 0.12485(0.12011: 20 °C), 0.12205(0.11713: 35 °C)	1954	CC	46
	0.1291(0.11912: 25 °C)	1957	PP	16
	0.1323(0.12011: 20 °C)	1957	CC	19
	0.1239(0.11813: 30 °C)	1960	PP&CC	37
	0.1256(0.12268: 7.05 °C), 0.1246(0.12204: 10.26 °C), 0.1179(0.11650: 38.20 °C)	1968	SHW	9
	0.2759(0.12011: 20 °C), 0.1220(0.11614: 40 °C), 0.1182(0.11217: 60 °C)	1971	CC	47
	0.1270(0.12173: 11.85 °C), 0.119(0.11458: 47.85 °C)	1976	CS	45
	0.1238(0.11912: 25 °C)	1982	RTHW	22
	0.1232(0.12018: 19.65 °C)	2002	THW	36
hemimellitene	0.1333(0.13172: 0 °C)	1969	THW	48
pseudocumene	0.1338(0.13069: 5.80 °C), 0.1323(0.12956: 11.68 °C), 0.1272(0.12512: 34.77 °C)	1968	SHW	9
	0.1303(0.12796: 20 °C), 0.12644(0.12412: 40 °C), 0.1223(0.12027: 60 °C)	1971	CC	47
mesitylene	0.136(0.13615: 20 °C)	1951	CC	40
	0.1440(0.13615: 20 °C)	1957	CC	19
	0.1337(0.13395: 30 °C)	1960	PP&CC	37
	0.1404(0.13937: 5.31 °C), 0.1396(0.13874: 8.18 °C), 0.1331(0.13264: 35.98 °C)	1968	SHW	9
	0.1370(0.13615: 20 °C), 0.1325(0.13175: 40 °C), 0.1280(0.12736: 60 °C)	1971	CC	47

<sup>a</sup> SHW, stationary hot-wire method; THW, transient hot-wire method; PP, parallel planes; CC, concentric cylinders; ACHR, AC heated rod; RTHW, relative transient hot-wire method; ACHW, AC heated-wire; TCC, transient concentric cylinder; CS, concentric spheres; PP&CC, joint technique of PP and CC.

Table 5. Present Data of the Thermal Conductivity, Thermal Diffusivity, Volumic, Massic, and Molar Heat Capacity at 298.15 K and 101.325 kPa, Together with Molar Mass, Boiling Point, Density, Temperature Dependence of Thermal Conductivity and Thermal Diffusivity, and Values of the Molar Heat Capacity Found in the Literature

material	<i>M</i> g·mol <sup>-1</sup>	<i>ϑ</i> <sub>b</sub> °C	<i>λ</i> W·m <sup>-1</sup> ·K <sup>-1</sup>	<i>a</i> 10 <sup>-8</sup> m <sup>2</sup> ·s <sup>-1</sup>	<i>c</i> <sub>p</sub> <i>ρ</i> MJ·m <sup>-3</sup> ·K <sup>-1</sup>	<i>c</i> <sub>p</sub> kJ·kg <sup>-1</sup> ·K <sup>-1</sup>	<i>C</i> <sub>m,p</sub> J·mol <sup>-1</sup> ·K <sup>-1</sup>	<i>ρ</i> kg·m <sup>-3</sup>	( <i>dλ/dT</i> )/ <i>λ</i> 10 <sup>-3</sup> K <sup>-1</sup>	( <i>da/dT</i> )/ <i>a</i> 10 <sup>-3</sup> K <sup>-1</sup>	<i>C</i> <sub>m,p</sub> J·mol <sup>-1</sup> ·K <sup>-1</sup>
1-pentene	70.135	29.96 <sup>a</sup>	0.11242	8.132	1.383	2.176	152.6	635.3 <sup>a</sup>	-3.50	-3.61	154.0 <sup>b</sup>
1-hexene	84.163	63.485 <sup>a</sup>	0.11732	8.205	1.430	2.139	180.0	668.48 <sup>a</sup>	-2.90	-3.04	183.3 <sup>b</sup>
2,3-dimethyl-1-butene	84.163	55.616 <sup>a</sup>	0.10478	7.274	1.440	2.140	180.1	673.25 <sup>a</sup>	-1.80	-2.55	
2,3-dimethyl-2-butene	84.163	73.205 <sup>a</sup>	0.12145	8.383	1.449	2.059	173.3	703.47 <sup>a</sup>	-2.93	-3.26	174.68 <sup>e</sup>
1-heptene	98.19	93.643 <sup>a</sup>	0.12130	8.314	1.459	2.106	206.8	692.67 <sup>a</sup>	-2.581	-2.77	211.8 <sup>b</sup>
1-octene	112.217	121.29 <sup>a</sup>	0.12387	8.049	1.539	2.163	243.0	710.9 <sup>a</sup>	-2.40	-3.21	241.2 <sup>b</sup>
cyclopentene	68.118	44.242 <sup>a</sup>	0.13180	9.705	1.358	1.772	120.7	766.53 <sup>a</sup>	-3.28	-4.13	122.4 <sup>b</sup>
cyclohexene	82.147	82.979 <sup>a</sup>	0.12737	8.870	1.436	1.781	146.3	806.09 <sup>a</sup>	-2.52	-3.46	148.35 <sup>f</sup>
cyclopentane	70.135	49.262 <sup>a</sup>	0.12637	9.458	1.336	1.804	126.6	740.45 <sup>a</sup>	-3.12	-4.42	126.78 <sup>g</sup>
cyclohexane	84.163	80.738 <sup>a</sup>	0.11817	8.219	1.438	1.858	156.4	773.89 <sup>a</sup>	-2.42	-3.74	156.5 <sup>b</sup>
cyclohexane- <i>d</i> <sub>12</sub>	96.253		0.11146	6.394	1.743	1.965	189.1	887.0 <sup>d</sup>	-2.38	-3.75	188.7 <sup>h</sup>
methylcyclopentane	84.163	71.812 <sup>a</sup>	0.11454	8.209	1.395	1.876	157.9	743.94 <sup>a</sup>	-2.78	-3.72	158.7 <sup>g</sup>
cycloheptane	98.190	118.79 <sup>a</sup>	0.11841	8.000	1.480	1.834	180.1	806.6 <sup>a</sup>	-2.05	-3.07	180.4 <sup>b</sup>
cyclooctane	112.217	151.14 <sup>a</sup>	0.11843	7.333	1.615	1.941	217.8	832.00 <sup>a</sup>	-1.80	-2.55	215.5 <sup>b</sup>
benzene	78.115	80.094 <sup>a</sup>	0.14081	9.432	1.493	1.709	133.5	873.66 <sup>a</sup>	-2.31	-2.22	135.95 <sup>a</sup>
benzene- <i>d</i> <sub>6</sub>	84.160		0.13425	7.845	1.711	1.815	152.7	943.0 <sup>d</sup>	-2.38	-2.49	152.46 <sup>i</sup>
1,3-cyclohexadiene	80.131	80.3 <sup>b</sup>	0.13252	8.956	1.480	1.763	141.3	839.2 <sup>d</sup>	-1.80	-2.55	141.3 <sup>j</sup>
1,4-cyclohexadiene	80.131	88.3 <sup>b</sup>	0.14474	9.463	1.529	1.796	144.0	851.4 <sup>d</sup>	-2.41	-2.96	142.2 <sup>j</sup>
toluene <sup>2</sup>	92.142	110.630 <sup>a</sup>	0.13051	9.060	1.441	1.671	154.0	862.2 <sup>a</sup>	-2.18	-2.26	157.29 <sup>a</sup>
toluene- <i>d</i> <sub>8</sub>	100.202		0.12471	7.537	1.655	1.764	176.8	937.9 <sup>d</sup>	-2.13	-2.82	
bicyclo[2.2.1]hepta-2,5-diene	92.142	89.5 <sup>c</sup>	0.13618	9.432	1.444	1.601	147.6	901.6 <sup>d</sup>	-2.30	-3.77	161.2 <sup>k</sup>
ethylbenzene	106.169	136.202 <sup>a</sup>	0.12752	8.649	1.502	1.741	184.9	862.60 <sup>a</sup>	-1.95	-2.40	185.96 <sup>a</sup>
1,2-dimethylbenzene	106.169	144.429 <sup>a</sup>	0.12875	8.429	1.527	1.743	185.1	875.9 <sup>a</sup>	-1.62	-2.23	188.07 <sup>a</sup>
1,3-dimethylbenzene	106.169	139.12 <sup>a</sup>	0.12943	8.967	1.443	1.678	178.2	860.0 <sup>a</sup>	-1.93	-2.45	183.44 <sup>a</sup>
1,4-dimethylbenzene	106.169	138.359 <sup>a</sup>	0.12679	8.724	1.453	1.696	180.1	856.7 <sup>a</sup>	-2.00	-2.53	181.66 <sup>a</sup>
<i>n</i> -propylbenzene	120.196	159.242 <sup>a</sup>	0.12772	8.434	1.514	1.765	212.2	857.90 <sup>a</sup>	-1.71	-2.19	214.71 <sup>a</sup>
(1-methylethyl)-benzene	120.196	152.411 <sup>a</sup>	0.11912	7.806	1.526	1.78	213.9	857.5 <sup>a</sup>	-1.67	-2.32	215.40 <sup>j</sup>
1,2,3-trimethylbenzene	120.196	176.117 <sup>a</sup>	0.12752	7.989	1.596	1.792	215.4	890.5 <sup>a</sup>	-1.32	-1.73	216.10 <sup>a</sup>
1,2,4-trimethylbenzene	120.196	169.378 <sup>a</sup>	0.12701	8.248	1.540	1.766	212.3	871.8 <sup>a</sup>	-1.51	-2.04	215.03 <sup>a</sup>
1,3,5-trimethylbenzene	120.196	164.743 <sup>a</sup>	0.13505	8.998	1.501	1.743	209.5	861.1 <sup>a</sup>	-1.63	-2.39	209.10 <sup>a</sup>

<sup>a</sup> Referred from TRC Table.<sup>7</sup> <sup>b</sup> Referred from Kagaku Binran.<sup>6</sup> <sup>c</sup> Héberger.<sup>50</sup> <sup>d</sup> Measured value. <sup>e</sup> Scott et al.<sup>51</sup> <sup>f</sup> Haida et al.<sup>52</sup> <sup>g</sup> Douslin et al.<sup>53</sup> <sup>h</sup> Mraw et al.<sup>54</sup> <sup>i</sup> Rabinovich et al.<sup>55</sup> <sup>j</sup> Steele et al.<sup>56</sup> <sup>k</sup> Steele.<sup>57</sup> <sup>l</sup> Kishimoto et al.<sup>58</sup>

correspondently with each original hydrogenated ones (cf. *Thermal Properties of Deuterated Liquids*).

Referring to the previous reports<sup>4,5</sup> and considering that the thermal conductivity of benzene agrees with the values by the IUPAC recommendation and that the correspondences between isomers (toluene/norbornadiene, or 1,3-/1,4-cyclohexadiene) and between deuterated and hydrogenated carbons (cyclohexane, benzene, and toluene), empirical equations for the thermal conductivity and thermal diffusivity of 29 hydrocarbons and deuterated ones in the liquid phase are reported, with an uncertainty of

Table 6. Comparisons between the Deuterated and Hydrogenated Carbons (the Values of Toluene C<sub>7</sub>H<sub>8</sub> Are Previously Obtained<sup>2</sup>)

	present results (at 25 °C)				Horrocks et al. <sup>20</sup>
	( <i>M</i> <sub>D</sub> / <i>M</i> <sub>H</sub> ) <sup>1/2</sup>	<i>λ</i> <sub>H</sub> / <i>λ</i> <sub>D</sub>	<i>a</i> <sub>H</sub> / <i>a</i> <sub>D</sub>	( <i>C</i> <sub>m,p</sub> ) <sub>H</sub> / ( <i>C</i> <sub>m,p</sub> ) <sub>D</sub>	
benzene	1.038	1.049	1.202	0.874	1.042 (at 20 °C)
toluene	1.043	1.047	1.202	0.871	
cyclohexane	1.069	1.060	1.285	0.827	1.063 (at 20 °C)

0.4% for the thermal conductivity and 1.8% for the thermal diffusivity and the heat capacity (respectively, with a level

$k_p = 2$ ,  $p = 95\%$ ), although that of the thermal conductivity (not for thermal diffusivity) may be inferior for hemimellitene containing comparatively more impurities (i.e., other isomers). A curious phenomenon was observed in the measurement of 1,3-cyclohexadiene in the temperature range of  $-16\text{ }^\circ\text{C}$  to  $20\text{ }^\circ\text{C}$ , but it is necessary to accurately determine the cause of this phenomenon. The present result is expected to be of use for estimating or predicting the unknown thermal properties of other materials.

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**Note Added after ASAP Posting.** This article was released ASAP on 5/21/2004. In the caption to Figure 7,  $J_0$  was changed to  $\vartheta_0$ . The paper was reposted 6/2/2004.

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