

TS1. Experimental and calculated diamagnetic susceptibilities of 720 organic compounds (training set)

No	compounds	$-\chi_M(10^{-6}\text{cgs})$			
		Exp.	Cal.1	Cal.2	Cal.3
1	acetaldehyde	22.70	26.89	28.77	29.19
2	acetamide	34.10	33.04	34.25	34.61
3	acetic acid	31.54	32.08	32.83	32.94
4	acetic anhydride	52.80	55.54	57.32	56.36
5	acetone	33.70	38.96	40.31	40.01
6	acetylene	12.50	16.97	17.15	17.66
7	n-amyl alcohol	67.50	66.46	66.24	66.44
8	isoamyl alcohol	68.96	66.22	65.62	65.86
9	tert-amyl alcohol	70.90	67.49	66.00	65.89
10	n-amylamine	69.40	67.67	67.94	68.49
11	isoamylamine	71.60	67.43	67.41	67.90
12	isoamyl bromide	88.70	89.53	92.04	89.68
13	isoamyl chloride	79.00	76.92	77.01	76.64
14	bromochloromethane	55.00	58.80	58.58	59.05
15	bromodichloromethane	66.30	69.14	67.81	68.39
16	bromotrichloromethane	73.10	79.22	77.18	77.85
17	butane	57.40	52.73	52.51	52.91
18	isobutane	51.70	51.87	51.44	51.29
19	n-butyl alcohol	56.54	55.47	54.97	55.33
20	isobutyl alcohol	57.70	55.24	54.22	54.57
21	sec-butyl alcohol	57.68	56.21	55.35	55.58
22	tert-butyl alcohol	57.42	55.40	54.15	53.31
23	n-butylamine	58.90	56.68	56.70	57.38
24	isobutylamine	59.80	56.44	55.88	56.70
25	isobutyl bromide	79.88	78.65	78.74	79.46
26	n-butyl chloride	67.10	66.17	66.01	66.12
27	carbon tetrachloride	66.60	69.48	66.56	67.24
28	carbon tetrabromide	93.73	105.02	105.49	109.72
29	chloroacetic acid	48.10	46.44	46.17	47.13
30	chloroacetone	50.90	53.32	53.77	54.36
31	chlorodibromomethane	75.10	79.36	78.87	79.91
32	chlorodifluoromethane	38.60	34.51	34.88	35.88
33	1-chloro-2,3-dihydroxypropane	77.90	61.99	60.04	60.67
34	chlorotrifluoromethane	45.30	39.69	37.17	38.22
35	cyclohexane	68.13	69.02	67.95	68.47
36	1,3-cyclohexadiene	48.60	58.27	57.63	58.36
37	1,4-cyclohexadiene	48.70	58.22	57.49	58.12
38	cyclohexanol	73.40	73.06	71.83	72.49
39	cyclohexanone	62.00	67.99	68.61	69.94
40	cyclohexene	57.50	63.62	62.83	63.54
41	cyclooctane	91.40	91.00	91.86	92.92
42	cyclooctene	84.60	85.60	86.20	87.25
43	cyclopentane	59.18	58.04	55.50	55.51
44	cyclopentanone	51.63	57.00	56.54	57.53
45	cyclopropane	39.90	36.06	27.63	26.96
46	dibromodichloromethane	81.10	88.39	87.22	88.48
47	1,2-dibromo-2-fluoroethane	78.00	82.37	83.95	83.85
48	1,2-dibromotetrachloroethane	126.00	128.17	124.95	126.83
49	1,1-dichlorodifluoroethylene	60.00	55.30	54.10	54.85
50	1,2-dichloro-1,2-dibromoethane	108.60	105.76	104.43	111.64
51	dichlorodifluoromethane	52.20	48.87	47.42	47.89
52	1,1-dichloroethylene	49.20	49.85	47.87	47.26
53	1,2-dichloro-2-hydroxypropane	80.10	71.95	69.30	69.85
54	dicyclohexyl	129.31	131.51	136.78	138.88
55	diethylamine	56.80	58.30	59.17	58.71
56	diethylcyclohexylamine	124.50	122.05	123.34	122.03
57	1,1-difluoro-2,2-dibromoethane	85.50	81.31	81.84	84.69
58	1,1-difluoro-2,2-dichloroethyl amyl ether	129.84	124.72	120.73	121.36
59	1,1-difluoro-2,2-dichloroethyl butyl ether	119.48	113.73	109.45	110.26

60	1,1-difluoro-2,2-dichloroethyl propyl ether	107.19	102.75	98.41	99.15
61	1,1-difluoro-2,2-dichloroethyl ethyl ether	96.13	91.78	87.59	88.04
62	1,1-difluoro-2,2-dichloroethyl methyl ether	80.68	80.00	75.58	75.75
63	di- <i>n</i> -heptylamine	171.50	168.13	170.54	169.77
64	di- <i>n</i> -hexylamine	148.90	146.16	148.14	147.56
65	dimethoxymethane	47.30	49.40	49.01	46.23
66	2,2-dimethylbutane	76.24	73.91	72.94	72.98
67	2,3-dimethylbutane	76.22	74.64	73.77	75.50
68	2,4-dimethyl-2,4-hexadiene	78.70	87.07	86.87	83.87
69	2,5-dimethyl-4-heptene	100.60	103.04	102.94	101.80
70	2,3-dimethylhexane	98.77	97.20	97.77	98.03
71	2,5-dimethylhexane	98.15	96.20	96.49	96.17
72	3,4-dimethylhexane	99.06	97.81	98.49	98.68
73	2,6-dimethyl-4-hexanol	116.90	100.48	100.86	99.83
74	2,4-dimethylnonane	134.68	129.76	131.79	130.07
75	3,4-dimethylnonane	134.70	130.76	132.21	131.88
76	4,5-dimethylnonane	134.52	130.75	132.51	131.76
77	2,6-dimethyloctane	122.54	118.79	119.70	119.27
78	2,2-dimethylpentane	86.97	84.88	85.40	83.90
79	2,3-dimethylpentane	87.51	86.23	86.29	87.04
80	2,4-dimethylpentane	87.48	85.21	86.32	84.88
81	2,2-dimethylpropane	63.10	61.81	60.98	60.38
82	ethane	27.30	31.63	32.10	31.90
83	ethyl alcohol	33.60	33.51	33.11	33.12
84	ethyl bromide	54.70	56.54	56.94	56.94
85	ethyl bromoacetate	82.80	83.53	85.22	83.65
86	ethyl <i>n</i> -butyrate	77.70	79.26	80.22	79.49
87	ethyl isobutyrate	78.32	79.72	80.04	79.28
88	ethyl chloroacetate	72.30	70.77	70.99	70.53
89	ethyl cyclohexane	91.09	91.94	92.19	92.34
90	ethyl dichloroacetate	85.20	84.08	83.27	83.13
91	ethyl iodide	69.70	68.20	68.28	65.92
92	ethyl propionate	66.50	68.30	69.15	68.42
93	ethyl tribromoacetate	119.50	125.07	126.44	124.60
94	ethyl trichloroacetate	99.60	96.57	94.68	94.07
95	fluorobromoacetic acid	59.50	59.35	60.42	60.57
96	fluorodichloromethane	48.80	46.12	45.73	46.37
97	formic acid	19.90	19.07	20.52	21.52
98	formamide	21.90	20.19	22.09	23.33
99	1,2-heptadiene	73.50	73.53	73.78	73.37
100	2,3-heptadiene	72.10	75.10	75.46	74.49
101	heptyldehyde	81.02	82.19	84.53	85.26
102	heptane	85.24	85.69	86.45	86.23
103	4-heptanol	91.50	89.73	90.03	89.43
104	<i>n</i> -heptanoic acid	88.60	87.90	89.03	89.40
105	<i>n</i> -heptylamine	93.10	89.64	90.34	90.70
106	heptylcyclohexane	147.40	146.86	148.23	147.77
107	1-heptyne	77.00	73.74	74.56	74.66
108	2-heptyne	79.50	75.24	76.17	75.36
109	hexabromoethane	148.00	165.00	165.51	149.82
110	hexachloroethane	112.70	108.04	102.88	105.61
111	<i>n</i> -hexane	74.60	74.70	75.25	75.12
112	<i>n</i> -hexyl alcohol	79.20	77.44	77.44	77.55
113	4-hydroxy-2-butanone	48.50	53.57	54.32	54.57
114	methyl acetate	42.60	44.62	45.29	44.09
115	methyl alcohol	21.40	22.15	21.54	20.95
116	methyl bromide	42.80	48.99	51.10	51.01
117	methylamine	27.00	23.54	23.54	23.53
118	2-methylbutane	64.40	63.49	62.98	63.64
119	2-methyl-2-butene	54.14	58.20	57.59	56.56
120	methyl chloride	32.00	34.46	34.29	34.56
121	methyl chloroacetate	58.10	58.99	58.97	58.23

122	methylcyclohexane	78.91	80.37	80.14	80.55
123	2-methylcyclohexanone	74.00	79.99	80.95	82.20
124	3-methylcyclohexanone	74.80	79.33	80.67	81.66
125	methylcyclopentane	70.17	69.38	67.92	67.93
126	methyl dichloroacetate	73.10	72.30	71.35	70.82
127	3-methylheptane	97.99	97.05	97.74	97.64
128	2-methylheptene	88.00	90.31	90.41	89.42
129	5-methyl-1,2-hexadiene	73.60	73.29	73.18	72.69
130	2-methylhexane	86.24	85.45	85.94	85.65
131	5-methyl-5-nonene	111.60	114.25	114.88	113.48
132	4-methyloctane	109.63	108.02	109.49	108.60
133	2-methylpentane	75.26	74.47	75.06	74.54
134	3-methylpentane	75.52	75.09	75.11	75.57
135	4-methyl-2-pentanol	80.40	77.93	78.06	76.98
136	2-methylpropene	44.40	45.56	44.85	43.84
137	methyl propionate	55.00	56.51	57.12	56.11
138	nitroethane	35.40	31.50	38.23	43.53
139	nitromethane	21.10	18.16	25.74	31.26
140	2-nitropropane	45.73	44.25	49.51	54.48
141	n-nonane	108.13	107.66	108.85	108.44
142	n-octane	96.63	96.68	97.65	97.34
143	octyl alcohol	102.65	99.42	99.84	99.76
144	octyl chloride	114.90	110.12	110.71	110.55
145	octylcyclohexane	158.09	157.85	159.43	158.87
146	pentachloroethane	99.10	95.57	91.43	94.93
147	2,3-pentadiene	49.10	52.81	53.13	51.74
148	n-pentane	63.05	63.72	64.12	64.02
149	2,4-pentanediol	70.40	70.65	69.99	69.08
150	propane	40.50	41.70	41.63	41.80
151	propene	31.50	34.37	33.76	33.34
152	propionaldehyde	34.32	38.26	39.93	40.83
153	propionic acid	43.50	43.97	44.35	45.01
154	propionitrile	38.50	36.86	38.92	39.67
155	n-propyl acetate	65.91	67.37	68.30	67.49
156	isopropyl acetate	67.04	67.79	68.71	67.14
157	n-propyl alcohol	45.18	44.48	43.83	44.23
158	isopropyl alcohol	45.79	44.62	43.95	43.62
159	isopropyl bromide	65.10	65.12	64.92	64.67
160	n-propyl bromide	65.60	67.79	68.13	68.05
161	isopropylcyclohexane	102.65	103.07	103.39	103.55
162	acetonitrile	28.00	25.21	27.42	27.72
163	acetyl chloride	38.90	41.09	41.86	41.73
164	alanine	50.50	49.18	48.87	49.82
165	allyl acetate	56.70	60.33	60.56	59.57
166	allyl alcohol	36.70	37.43	36.25	36.30
167	n-amyl acetate	89.06	89.34	90.63	89.70
168	isoamyl acetate	89.40	89.11	89.96	89.12
169	isoamyl n-butyrate	113.52	111.97	112.70	112.23
170	isoamyl cyanide	73.40	69.57	71.62	72.41
171	isoamyl ether	129.00	122.73	122.70	121.82
172	n-amyl methyl ketone	80.50	83.79	85.66	85.47
173	isoamyl propionate	101.73	101.00	101.63	101.15
174	bromoform	82.60	88.93	89.24	91.44
175	n-butyl acetate	77.47	78.36	79.35	78.60
176	isobutyl acetate	78.52	78.13	78.78	77.80
177	2-n-butyl chloride	67.40	65.67	64.56	65.59
178	n-butyl cyanide	62.80	58.82	60.97	61.89
179	tert-butylcyclohexane	115.09	113.80	113.90	113.14
180	n-butyl ethyl ketone	80.73	84.67	86.26	86.44
181	n-butyl formate	65.83	65.12	66.78	67.03
182	isobutyl formate	66.79	64.88	66.27	66.24
183	isobutyl methyl ketone	70.05	72.56	74.31	73.60

184	<i>tert</i> -butyl methyl ketone	69.86	73.20	73.00	73.17
185	<i>n</i> -butyric acid	55.10	54.94	55.51	56.08
186	isobutyric acid	56.06	55.39	55.14	55.91
187	butyronitrile	49.40	47.83	49.85	50.78
188	chloroform	59.30	58.28	56.05	56.87
189	cyclohexanecarboxylic acid	83.24	83.82	83.61	84.55
190	cyclooctatetraene	53.90	70.39	69.50	70.00
191	diisobutylamine	133.10	123.71	124.47	124.18
192	di- <i>n</i> -butylamine	103.70	102.21	103.23	103.13
193	diisobutylamine	105.70	101.74	102.29	101.67
194	di- <i>sec</i> -butylamine	105.90	104.03	104.65	103.90
195	diisobutyl ketone	104.30	106.15	107.90	107.10
196	<i>n</i> -amyl nitrate	76.40	71.23	76.99	81.33
197	<i>n</i> -butyl bromide	77.14	78.78	80.57	79.15
198	<i>n</i> -butyl iodide	93.60	90.63	92.75	88.13
199	<i>n</i> -butyl sulfide	113.70	122.24	123.87	108.44
200	<i>n</i> -butyl thiocyanate	79.38	83.81	85.14	72.99
201	di- <i>tert</i> -butyl ketone	104.06	107.46	108.06	105.35
202	1,1-dicyclohexylnonane	231.98	231.70	239.55	239.97
203	diethyl ketone	58.10	62.72	64.09	64.28
204	diethyl sulfide	67.90	77.98	77.34	64.02
205	dimethyl sulfide	44.90	59.56	58.27	41.80
206	1,4-dioxane	52.16	56.15	55.98	56.13
207	di- <i>n</i> -propyl ketone	80.45	84.65	86.44	86.39
208	diisopropyl ketone	81.14	85.50	86.66	86.19
209	diethyl ether	55.10	57.32	57.66	56.35
210	ethyl formate	43.00	43.16	44.82	44.82
211	ethyl <i>n</i> -propyl ketone	69.03	73.69	75.24	75.34
212	ethyl thiocyanate	55.70	61.68	61.85	50.78
213	<i>n</i> -hexyl methyl ketone	91.40	94.78	96.86	96.57
214	methyl butyl ketone	69.10	72.80	74.40	74.36
215	dimethyl ether	26.30	33.80	33.50	31.68
216	methyl ethyl ketone	45.50	50.85	51.95	52.22
217	methyl <i>n</i> -propyl ketone	57.41	61.81	63.43	63.26
218	methyl isopropyl ketone	58.45	62.24	62.79	63.48
219	<i>n</i> -propyl iodide	84.30	79.65	79.69	77.02
220	1,1,2,2-tetrabromoethane	123.40	126.87	127.38	144.21
221	1,1,2,2-tetrachloroethane	89.80	83.35	80.11	83.99
222	1,2,3-tribromopropane	117.90	119.02	122.65	122.09
223	trichloronitromethane	75.30	62.27	64.42	69.33
224	triethylamine	81.40	82.05	83.58	82.41
225	2,2,3-trimethylbutane	88.36	85.36	83.93	85.29
226	2,2,3-trimethylpentane	99.86	96.95	96.76	96.69
227	1,2-dichloro-1,1,2-trifluoroethane	66.20	62.97	60.93	62.68
228	1,2-dibromo-1,1,2-trifluoroethane	90.90	85.43	85.79	86.17
229	1-methoxy-1,1,2-trifluoroethane	55.90	52.59	50.61	50.83
230	1-chloro-2-propene	47.80	48.16	46.83	47.09
231	1-bromo-2-propene	58.60	60.87	60.78	60.12
232	1-iodo-2-propene	72.80	72.84	72.45	69.10
233	1-amine-2-propene	40.10	38.64	37.91	38.34
234	benzene	54.84	53.57	52.45	53.08
235	fluorobenzene	58.40	55.98	55.48	56.52
236	phenol	60.21	58.63	56.98	57.42
237	benzaldehyde	60.78	63.50	63.82	64.87
238	nitrobenzene	61.80	59.61	62.55	67.93
239	aniline	62.95	59.65	58.45	59.13
240	benzonitrile	65.19	62.38	62.91	63.91
241	<i>p</i> -nitrosonitrobenzene	65.80	64.37	70.95	77.23
242	<i>m</i> -nitrosonitrobenzene	66.00	64.38	70.98	77.21
243	toluene	66.11	65.80	64.77	64.68
244	<i>p</i> -nitroaniline	66.43	65.70	68.50	73.96
245	<i>o</i> -nitroaniline	66.47	66.12	68.64	74.11

246	<i>p</i> -nitrobenzaldehyde	66.57	69.55	73.87	79.70
247	phenylhydrazine	67.82	65.33	64.95	65.59
248	phenylhydroxylamine	68.20	64.15	63.45	63.91
249	<i>o</i> -nitrobenzaldehyde	68.23	69.96	74.03	79.84
250	<i>m</i> -nitrobenzaldehyde	68.55	69.55	73.90	79.68
251	<i>p</i> -nitrophenol	69.50	64.68	67.03	72.25
252	chlorobenzene	69.97	67.98	66.38	66.44
253	<i>m</i> -nitroaniline	70.09	65.70	68.55	73.94
254	benzoic acid	70.28	69.81	68.53	69.28
255	<i>m</i> -nitrophenol	70.80	64.68	67.06	72.23
256	phenylthiol	70.80	74.78	71.33	61.72
257	benzyl alcohol	71.83	69.33	67.66	67.95
258	acetophenone	72.05	76.62	76.42	76.55
259	<i>p</i> -toluidine	72.10	71.89	70.69	70.72
260	benzamide	72.30	70.84	70.02	70.99
261	2,4-dinitrophenol	73.10	71.15	77.19	87.17
262	<i>o</i> -nitrophenol	73.30	65.10	67.15	72.38
263	1,3,5-trinitrobenzene	74.55	71.72	82.67	97.51
264	<i>m</i> -toluidine	74.60	71.89	70.89	70.68
265	benzylamine	75.26	70.53	69.38	70.02
266	benzoyl chloride	75.60	78.89	78.05	78.30
267	<i>o</i> -methoxybenzaldehyde	76.00	81.36	81.27	80.44
268	<i>o</i> -toluidine	76.00	72.17	70.85	71.02
269	<i>o</i> -nitrobenzoic acid	76.11	76.27	78.74	84.22
270	<i>m</i> -xylene	76.56	78.04	77.34	76.22
271	<i>p</i> -xylene	76.78	78.04	76.98	76.27
272	<i>o</i> -aminobenzoic acid	77.18	76.20	74.69	75.47
273	ethylbenzene	77.20	77.58	76.76	76.75
274	<i>o</i> -chlorophenol	77.40	73.34	70.99	71.03
275	<i>p</i> -chlorophenol	77.60	73.04	70.82	70.76
276	<i>o</i> -xylene	77.68	78.30	77.18	76.76
277	<i>p</i> -methoxybenzaldehyde	78.00	81.05	81.01	80.31
278	<i>p</i> -nitrobenzoic acid	78.81	75.85	78.58	84.11
279	bromobenzene	78.92	79.29	78.79	77.34
280	<i>m</i> -anisidine	79.95	77.21	75.72	74.55
281	<i>m</i> -chlorotoluene	80.07	80.22	78.99	77.98
282	<i>p</i> -chlorotoluene	80.07	80.21	78.58	78.02
283	<i>m</i> -nitrobenzoic acid	80.22	75.86	78.60	84.09
284	<i>o</i> -anisidine	80.44	77.52	75.87	74.71
285	<i>p</i> -anisidine	80.56	77.20	75.65	74.57
286	phenyl isothiocyanate	81.50	78.63	79.13	72.57
287	benzyl chloride	81.98	80.06	78.64	78.88
288	<i>o</i> -chlorotoluene	81.98	80.48	78.80	78.58
289	<i>p</i> -dichlorobenzene	82.93	82.39	80.19	79.78
290	<i>m</i> -dichlorobenzene	83.19	82.40	80.64	79.73
291	<i>o</i> -chlorobenzoic acid	83.56	84.50	82.76	82.89
292	<i>p</i> -bromoaniline	84.06	85.38	84.64	83.37
293	<i>o</i> -dichlorobenzene	84.26	82.66	80.41	80.41
294	picric acid	84.38	77.64	87.33	102.04
295	<i>m</i> -bromoaniline	84.89	85.38	85.05	83.31
296	<i>p</i> -dimethoxybenzene	86.65	88.66	86.91	83.98
297	<i>m</i> -dimethoxybenzene	87.21	88.67	86.93	83.96
298	<i>o</i> -bromonitrobenzene	87.30	85.76	89.14	92.56
299	<i>o</i> -bromoaniline	87.32	85.69	84.90	83.91
300	<i>o</i> -dimethoxybenzene	87.39	88.99	87.14	84.08
301	<i>m</i> -bromonitrobenzene	89.50	85.34	88.93	92.11
302	<i>p</i> -bromonitrobenzene	89.60	85.33	88.76	92.17
303	iodobenzene	92.00	89.98	89.16	84.84
304	benzyl acetate	93.18	92.23	91.97	91.21
305	<i>m</i> -bromotoluene	93.40	91.53	91.65	88.85
306	<i>n</i> -butylbenzene	100.79	99.54	98.99	98.90
307	<i>p</i> -iodotoluene	101.31	102.22	101.27	96.42

308	<i>p</i> -dibromobenzene	101.40	105.01	104.90	101.57
309	isobutylbenzene	101.81	99.30	98.72	98.14
310	<i>tert</i> -butylbenzene	102.50	99.81	98.28	97.46
311	biphenyl	103.25	103.22	102.30	103.24
312	diphenyl ether	108.10	108.52	107.13	107.56
313	benzophenone	109.60	114.40	113.71	115.01
314	diphenylamine	109.70	108.21	107.97	109.47
315	<i>n</i> -amylbenzene	112.55	110.53	110.24	110.01
316	diphenylmethane	115.70	113.39	112.99	113.76
317	hexamethylbenzene	122.50	128.59	127.97	124.82
318	pentabromophenol	194.00	189.19	193.39	185.18
319	1,2,5,6-dibenzofluorene	184.00	179.41	178.80	180.75
320	acenaphthene	109.30	107.32	107.98	109.94
321	acenaphthylene	111.60	102.71	102.19	104.08
322	anthracene	130.00	119.24	118.38	120.03
323	chrysene	166.67	152.66	151.45	153.12
324	dibenzopyrene	213.60	202.42	200.85	202.99
325	fluoranthene	138.00	136.14	135.25	137.16
326	fluorene	110.50	113.15	113.12	114.87
327	perylene	166.80	169.28	168.10	170.07
328	<i>p</i> -terphenyl	152.00	152.87	151.35	152.14
329	pyranthrene	266.90	251.58	249.74	252.60
330	tetracene	168.00	152.08	150.96	152.83
331	triphenylene	156.60	152.96	151.73	153.22
332	violanthrene	273.50	289.06	288.23	291.17
333	cyclobutane	40.00	47.05	40.92	41.78
334	1,2-dimethylcyclopentane	81.31	81.12	80.41	80.94
335	3,3-dimethylpentane	89.50	85.99	85.42	85.56
336	2,2,4-trimethylpentane	98.34	95.63	96.89	94.19
337	3-methyl-3-ethylpentane	99.90	98.06	98.41	97.98
338	<i>trans</i> -decahydronaphthalene	107.60	109.53	114.13	116.29
339	4-methylnonane	121.39	119.01	120.72	119.71
340	tridecane	153.70	151.61	153.65	152.87
341	tetradecane	166.20	162.60	164.85	163.97
342	2,2,4,7,9,9-hexamethyldecane	191.52	183.67	186.67	181.47
343	ethylene	18.80	22.43	21.60	21.50
344	1,3-butadiene	32.10	38.66	37.56	37.29
345	1-butene	41.00	45.69	45.02	44.98
346	<i>trans</i> -2-butene	43.30	46.71	46.28	45.42
347	cyclopentadiene	44.50	47.28	45.97	46.43
348	1,5-hexadiene	55.10	60.60	59.54	59.27
349	2,3-dimethyl-2-butene	65.90	69.95	69.05	68.51
350	fulvene	48.00	53.27	51.82	51.98
351	1-heptene	77.80	78.64	78.58	78.30
352	1-octene	88.80	89.62	89.78	89.41
353	isoamylene	53.70	56.69	55.68	55.65
354	phenylacetylene	72.01	66.20	65.26	65.59
355	isopropenylbenzene	80.00	82.98	81.22	80.56
356	propylbenzene	89.10	88.55	87.98	87.79
357	isopropylbenzene[Cumene]	89.50	88.90	87.86	87.81
358	dihydronaphthalene	85.10	91.06	91.43	93.00
359	4-phenyl-1-butene	93.49	92.48	91.18	90.97
360	1,2,3,4-tetrahydronaphthalene	93.30	96.15	97.34	99.08
361	d-limonene	98.00	103.70	103.38	102.58
362	1-methylnaphthalene	102.90	98.91	98.33	98.81
363	diisopropylbenzene	124.77	124.52	123.97	122.55
364	1,1-diphenylethylene	118.00	120.43	118.77	119.07
365	<i>m,m'</i> -bitolyl	127.40	127.70	126.92	126.04
366	diphenyldiacetylene	134.60	128.10	128.17	128.68
367	(<i>E</i>)-1-benzylidene-1H-indene	130.50	136.06	134.92	136.05
368	9-ethyl anthracene	153.00	143.83	143.40	143.80
369	1-phenyl-4,6,6-trimethylheptane	173.90	165.01	166.04	163.18

370	9-butylidene-9H-fluorene	147.50	155.18	154.49	155.01
371	<i>o</i> -terphenyl	150.40	153.17	151.66	152.24
372	diphenylhexatriene	146.90	154.02	152.18	151.25
373	9-butyl anthracene	176.00	165.78	165.47	165.97
374	1,6-Diphenylhexane	171.81	168.32	169.02	169.40
375	triphenylmethane	165.60	162.89	162.10	162.50
376	sugar	189.10	185.19	178.50	177.89
377	methylcholanthrene	182.00	185.51	185.81	187.32
378	3-methylcholanthrene	194.00	186.08	186.23	187.58
379	7-phenylbenzofulvene	131.00	136.56	135.21	135.91
380	4,4'-diphenylbiphenyl	201.30	202.52	200.37	201.01
381	1,1,4,4-tetraphenylbuta-1,2,3-triene	227.00	232.36	230.09	229.86
382	tetraphenylhexatriene	246.40	254.14	250.90	249.14
383	tetraphenyloctatetraene	264.10	270.76	267.36	265.17
384	trichlorofluoromethane	58.70	58.79	57.22	57.56
385	fluoromethane	17.80	18.45	19.51	19.57
386	triiodomethane	117.10	113.83	113.84	115.23
387	tetraiodomethane	136.00	131.52	132.57	138.96
388	tetrachloroethylene	81.60	78.54	75.16	76.16
389	fluoro trichloroethylene	72.50	66.51	64.86	65.22
390	1,2-dibromoethane	78.90	82.85	83.75	83.19
391	<i>trans</i> -1,2-dichloroethylene	48.90	51.48	49.64	49.14
392	chloroethylene	35.90	36.75	35.43	35.20
393	1,2-dichloroethane	59.60	57.63	56.10	57.12
394	trifluoroethene	32.20	27.87	29.93	31.53
395	2-chloropropene	47.80	47.71	46.37	45.55
396	1,4-dichloro-2-butene	74.20	69.84	69.56	69.31
397	amylidene chloride	93.40	89.79	89.19	89.51
398	amyl iodide	118.75	101.62	103.45	99.23
399	amylene bromide	114.50	106.26	106.97	104.84
400	1,1,1-tri(chloromethyl)ethane	114.00	105.47	104.30	104.52
401	octylene bromide	150.40	148.77	152.46	149.82
402	ethylene glycol	38.90	36.24	35.14	35.55
403	1,3-propylene glycol	50.20	47.22	46.08	46.65
404	erythritol	73.80	66.70	63.97	64.34
405	2,3-dibromo-2-butene-1,4-diol	94.20	103.94	102.78	101.75
406	2-butene-1,4-diol(cis)	54.30	52.82	51.51	51.34
407	tetrahydrofurfuryl alcohol	69.40	66.90	65.43	65.63
408	furfuryl alcohol	61.00	57.24	55.98	56.05
409	1,6-hexanediol	84.30	80.18	79.62	79.97
410	diisobutylmethanol	116.90	111.22	111.70	110.23
411	1-hexadecanol	183.50	187.31	189.44	188.61
412	formaldehyde	18.60	14.04	15.90	16.80
413	iso-butyraldehyde	46.38	49.32	50.56	51.33
414	iso-valeraldehyde	57.50	59.98	61.46	62.37
415	hexanal	69.40	71.20	73.33	74.15
416	phenylacetaldehyde	72.01	74.06	74.79	75.69
417	1,1-di(ethyloxycarbonyl)cyclopropane	110.40	116.07	110.18	108.16
418	methylacetylacetone	65.00	71.79	74.40	74.49
419	pentachlorohexadione	129.50	140.45	137.71	138.41
420	2-phenyl-5,7-dimethylpleiapentalene	179.00	177.43	176.50	176.09
421	dimethylcyclohexanone	84.80	91.44	92.19	92.87
422	thioglycollic acid	50.00	54.13	51.76	41.44
423	trichloroacetic acid	73.00	72.23	69.65	70.71
424	cyanuric acid	61.50	58.61	56.99	58.56
425	perfluoropropionic acid	61.00	61.33	54.87	57.73
426	chlorofumaric acid	67.02	67.36	66.62	66.89
427	tetronic acid	52.50	50.58	51.73	53.33
428	maleic acid	49.60	52.58	52.83	53.54
429	succinic acid	58.00	57.15	58.07	59.26
430	perfluoro- <i>n</i> -butyric acid	81.00	79.75	70.71	74.21
431	iso-valeric acid	67.70	65.69	66.19	66.44

432	uric acid	66.20	74.57	77.48	83.80
433	cyclobutanecarboxylic acid	58.16	61.85	57.50	58.68
434	hexanoic acid	78.10	76.91	77.83	78.30
435	Gallic acid	90.00	85.66	82.23	82.42
436	<i>cis</i> -9-octadecenoic acid	208.50	203.36	206.04	205.15
437	cholic acid	282.30	276.85	287.56	287.25
438	methyl formate	31.10	31.39	32.89	32.49
439	methyl trichloroacetate	84.20	84.79	82.84	81.75
440	methyl bromoacetate	77.10	71.75	73.28	71.35
441	ethyl-iso-cyanate	45.60	39.46	43.34	44.37
442	vinyl acetate	46.40	49.43	49.96	48.99
443	ethyl oxamate	62.00	61.68	62.48	62.70
444	propyl formate	55.00	54.13	55.74	55.93
445	ethyl thionacetate	63.50	68.41	68.78	60.29
446	diethyl carbonate	75.40	74.02	74.14	72.64
447	methyl perfluor- <i>n</i> -butyrate	92.50	92.31	83.40	85.28
448	methyl methacrylate	57.30	62.13	61.56	59.84
449	ethyl acetoacetate	71.70	77.37	79.47	78.66
450	dimethyl succinate	81.50	82.23	83.40	81.46
451	ethyl perfluor- <i>n</i> -butyrate	103.50	104.09	95.38	97.59
452	diethyl malonate	92.60	94.82	96.38	94.93
453	ethyl 3-methylbutanoate	91.10	90.01	90.86	89.86
454	1-butene-3,4-diyl diacetate	95.50	98.81	99.68	97.38
455	ethyl ethylacetoacetate	93.90	101.62	103.58	102.34
456	butane-1,4-diyl diacetate	103.40	103.99	106.01	104.29
457	dipropyl oxalate	105.27	107.03	107.31	106.61
458	hexyl acetate	100.90	100.33	101.83	100.81
459	<i>n</i> -butyl perfluor- <i>n</i> -butyrate	126.70	126.05	117.28	119.81
460	diethyl ethylmalonate	115.20	119.10	120.26	118.42
461	ethyl diethylmalonate	140.40	143.75	144.41	141.72
462	diethyl allylmalonate	118.80	123.02	123.53	121.52
463	ethyl diethylacetoacetate	117.90	126.24	127.89	125.78
464	<i>n</i> -amyl valerate	124.55	123.19	124.44	123.92
465	geraniol formate	119.90	121.45	123.05	120.53
466	4-ethoxy-3-methoxybenzyl acetate	138.50	139.44	138.64	134.45
467	propyl hexylpropiolate	136.80	136.21	137.56	136.66
468	ethylene oxide	30.50	29.63	25.12	24.65
469	ethyl vinyl ether	47.90	50.32	50.12	48.97
470	dipropyl ether	79.40	79.26	79.48	78.57
471	1,1-di(ethyloxycarbonyl)cyclobutane	118.00	127.05	123.54	121.88
472	1,2-ethanediamine	46.50	38.65	38.43	39.63
473	propylenediamine	58.10	50.22	49.69	50.66
474	camphane amine	122.00	117.63	120.80	122.32
475	tri- <i>iso</i> -amylamine	192.00	180.16	181.49	180.37
476	tri- <i>n</i> -heptylamine	251.30	246.80	250.83	248.76
477	chloroacetylchloride	53.70	55.47	55.34	56.11
478	butyryl chloride	62.10	63.96	65.07	64.99
479	2-ethylbutyrylchloride	87.20	87.54	89.14	88.58
480	difluoroacetamide	41.20	37.03	37.77	39.85
481	thioacetamide	42.45	45.23	45.17	38.43
482	succinimide	47.30	52.22	53.50	55.63
483	ethyl succinimide	72.00	75.80	77.41	79.24
484	maleic anhydride	35.80	47.08	47.40	49.04
485	glutamic acid	78.50	73.92	74.33	75.79
486	<i>iso</i> -leucine	84.90	83.47	83.34	84.35
487	acetoxime	44.42	32.97	35.10	35.13
488	<i>iso</i> -butyraldoxime	56.10	55.34	57.16	57.28
489	diethyl ketoxime	68.30	68.70	70.66	70.29
490	cyclohexanone oxime	71.50	73.97	75.14	75.94
491	<i>n</i> -hexyl methyl ketoxime	102.58	100.79	103.26	102.60
492	acetophenone oxime-O-methyl ether	92.31	95.37	95.62	93.58
493	acetoxime-O-benzyl ether	104.80	93.42	94.26	93.32

494	cytidine	123.70	128.18	126.58	129.32
495	2,6-dimethylpyridine	72.50	74.11	74.38	73.73
496	2,4,6-trimethylpyridine	83.10	86.36	87.08	85.18
497	tetraiodopyrrole	188.90	189.13	194.32	177.49
498	1-methylpyrrole	58.56	52.92	53.50	54.10
499	2,4-dimethylpyrrole	69.64	65.96	66.37	66.03
500	2,5-Dimethylpyrrole	71.92	66.37	66.51	66.09
501	1-allylpyrrole	73.80	69.12	68.95	69.47
502	2,5-dimethyl-3-ethyl-pyrrole	93.87	90.69	91.30	90.06
503	pyrazine	37.80	43.54	46.06	47.88
504	hexachlorobenzene	147.00	141.67	138.01	136.01
505	phenylfluoroform	77.30	76.33	71.39	72.95
506	benzylidene chloride	97.90	93.27	91.15	91.74
507	<i>o</i> -iodotoluene	112.20	102.55	101.62	97.61
508	1-chloronaphthalene	107.60	101.09	99.98	100.59
509	4,4'-dichlorobiphenyl	133.10	132.05	129.80	129.62
510	chlorodiphenylmethane	131.90	128.14	127.18	127.84
511	1,1-diphenylallyl-3-chloride	146.10	145.38	144.04	143.45
512	1,3-diphenylallyl-3-chloride	140.70	144.94	143.62	143.46
513	nitrophenyl fluoroform	84.10	82.79	81.61	87.88
514	2-nitrobiphenyl	109.00	109.68	112.40	118.02
515	5-nitroacenaphthylene	116.00	109.18	112.25	118.87
516	<i>m</i> -dinitrobenzene	70.53	65.66	72.62	82.74
517	nitrosobenzene	59.10	58.33	60.90	62.40
518	<i>m</i> -nitrotoluene	72.70	71.85	74.88	79.48
519	<i>p</i> -nitrotoluene	73.30	71.85	74.80	79.51
520	benzylidenemethylamine	73.10	76.26	75.16	75.26
521	benzylideneaminoethane	85.50	89.41	89.73	89.65
522	N-nitrosodiphenylamine	110.70	114.45	116.80	119.03
523	benzidine	110.90	115.39	114.00	115.00
524	<i>p</i> -phenylenediamine	70.70	65.74	64.39	65.17
525	<i>o</i> -phenylenediamine	72.50	66.04	64.52	65.37
526	azulene	91.00	86.40	85.77	87.13
527	N,N-dimethylaniline	85.10	83.81	83.09	82.24
528	N-ethylaniline	85.60	83.74	83.22	82.97
529	phthalimide	78.40	80.82	81.56	85.04
530	N,N-diethylaniline	107.90	107.98	107.87	106.68
531	1-naphthalenamine	92.50	92.78	91.86	93.17
532	N-1-naphthylacetamide	117.80	115.82	116.25	116.71
533	benzylidene aniline	100.40	115.39	115.16	116.31
534	N-phenylbenzothioamide	123.00	132.28	131.77	125.27
535	methylbenzylaniline	132.20	131.73	131.55	131.50
536	cinnamylideneaniline	123.20	132.19	131.75	132.37
537	1-chloro-2,4-dinitrobenzene	84.40	80.47	86.64	96.30
538	1-chloro-4-nitrobenzene	74.70	74.03	76.40	81.27
539	1-chloro-3-nitrobenzene	77.20	74.03	76.49	81.23
540	biphenylene	88.00	103.01	102.13	104.22
541	stilbestrol	130.00	129.88	127.31	127.46
542	<i>p</i> -methyl- <i>o</i> - <i>tert</i> -butyl-phenol	120.30	117.42	115.43	113.38
543	guaiacol	79.20	76.50	74.36	72.98
544	<i>p</i> -hydroquinone	64.70	63.69	61.45	61.75
545	1,4-diphenylbutadiene	130.00	136.57	135.10	135.16
546	trifluoro cresol	83.80	79.60	78.66	79.65
547	eugenol	102.10	104.44	101.91	99.68
548	<i>p</i> - <i>tert</i> -butylphenol	108.00	104.87	102.75	101.79
549	1-nitronaphthalene	98.47	92.86	95.87	101.92
550	4-nitroso-1-naphthol	91.80	96.86	98.83	100.71
551	1-(<i>o</i> -chloro phenylazo)-2-naphthol	161.00	164.43	163.31	164.44
552	1,3,5-cyclooctatriene	65.10	74.90	74.98	75.72
553	1-phenylazo-2-naphthol	137.60	149.70	149.32	150.99
554	1-(<i>o</i> -Methoxyphenylazo)-2-naphthol	163.60	167.60	166.62	166.39
555	diethylstilbestrol	172.00	178.75	177.12	174.96

556	1,3-cyclooctadiene	72.80	80.25	80.60	81.57
557	cinnamyl alcohol	87.20	86.20	84.38	84.09
558	diphenylmethanol	119.10	118.66	116.97	117.69
559	triphenylcarbinol	175.70	169.56	166.30	166.48
560	<i>o</i> -methoxybenzyl alcohol	87.90	87.18	85.16	83.54
561	phenetole	84.50	82.90	81.77	80.84
562	<i>p</i> -cresylmethyl ether	79.13	83.35	81.94	80.12
563	<i>m</i> -phenetidine	90.28	88.99	87.79	86.85
564	<i>p</i> -fluorophenetole	88.00	85.31	84.76	84.26
565	salicylaldehyde	66.80	68.87	68.45	69.35
566	<i>p</i> -hydroxybenzaldehyde	66.80	68.56	68.29	69.19
567	diphenyl acetic acid	124.50	129.38	128.83	129.61
568	<i>o</i> -(2,5-dimethoxybenzoyl)-benzoic acid	161.00	166.36	164.38	161.82
569	isophthalic acid	84.60	86.06	84.61	85.44
570	benzeneacetic acid	82.40	79.78	79.30	79.79
571	<i>m</i> -toluic acid	83.00	82.05	80.94	80.83
572	<i>o</i> -toluic acid	84.30	82.32	81.12	81.11
573	cinnamic acid	78.36	86.08	85.01	85.19
574	2-benzylidenemalononic acid	97.50	102.74	101.04	101.30
575	caproylphenylacetylene	130.40	134.01	134.51	134.44
576	chalcone	125.70	130.86	130.06	130.95
577	benzyl methyl ketone	83.44	86.65	87.15	86.94
578	benzoyl acetone	95.00	97.57	98.55	98.76
579	dimethylacetophenone	96.80	99.90	99.32	99.41
580	carvone	92.20	103.63	103.96	103.89
581	acetylphenylacetylene	86.90	89.18	89.39	89.10
582	propionylphenylacetylene	95.10	101.07	101.06	101.15
583	butyrylphenylacetylene	106.40	112.03	112.20	112.22
584	diphenylmethanethione	118.10	126.30	125.57	119.07
585	ethylallyl acetophenone	122.50	126.57	126.09	125.83
586	xanthone	108.10	119.52	118.40	120.33
587	benzil	106.80	125.58	125.14	126.80
588	dibenzyl ketone	131.70	134.33	135.19	136.08
589	diethylallylacetophenone	146.20	151.00	150.65	149.06
590	tri allyl acetophenone	152.50	158.83	157.24	155.04
591	3,7,7-trimethyl-1,3,5-cycloheptatriene	95.60	99.40	98.78	97.76
592	dibenzphenanthrone	200.50	190.64	190.50	192.62
593	phenyl iso-cyanate	72.70	65.34	67.42	68.74
594	phenyl thiocyanate	81.50	85.36	85.14	74.52
595	benzyl formate	81.43	78.99	79.46	79.64
596	phenyl acetate	82.04	82.03	81.53	80.82
597	methyl- <i>m</i> -hydroxybenzoate	88.40	87.43	85.75	84.65
598	methyl phenylacetate	92.73	92.32	91.89	90.90
599	phenyl propionate	93.79	93.93	93.12	92.86
600	methyl- <i>p</i> -methoxybenzoate	98.60	99.91	98.41	95.78
601	ethyl <i>p</i> -toluenesulfonate	115.00	116.88	112.78	113.19
602	ethyl phenylacetate	104.27	104.10	103.96	103.21
603	phenyl <i>n</i> -butyrate	105.46	104.89	104.22	103.93
604	methyl phenylpropionate	95.60	94.96	94.17	93.05
605	ethyl phenylpropionate	104.20	106.74	106.19	105.37
606	ethyl cinnamate	107.50	110.41	109.63	108.59
607	ethyl nitrophenylpropionate	114.60	119.92	124.14	128.38
608	<i>n</i> -butyl benzoate	116.69	116.10	115.09	114.87
609	ethyl benzylidenecyanoacetate	116.30	119.65	120.07	119.32
610	diethyl phthalate	127.50	135.03	134.13	132.34
611	ethyl methylphenylmalonate	153.20	157.66	156.27	153.89
612	phenylbutyl acetate	134.50	125.17	125.62	124.59
613	phenyl benzoate	117.30	119.78	118.58	119.40
614	methyl- <i>o</i> -benzoylbenzoate	139.40	143.50	142.57	142.23
615	dibutyl phthalate	175.10	178.94	177.92	176.77
616	4-ethoxy-3-methoxybenzyl benzoate	177.30	177.19	175.62	172.73
617	diethylstilbestrol dipropionate	265.20	249.35	249.41	245.83

618	rhamnose	99.20	88.36	86.91	87.24
619	bromobenzene diazo cyanide	86.88	95.91	99.75	99.27
620	xylose	84.80	76.23	74.82	75.63
621	N-phenyl urea	82.10	76.04	75.96	77.25
622	N-phenylthiourea	87.40	88.70	87.96	81.11
623	phenylacetylchloride	88.50	88.80	88.77	88.67
624	coumarin	82.50	85.89	85.66	87.31
625	safrole	97.50	101.88	100.62	100.65
626	Benzoic anhydride	134.90	131.03	130.06	131.24
627	borneol	126.00	116.59	119.11	120.33
628	3-bromo-7-hydroxy-4-methyl-2H-chromen-2-one	127.30	129.87	129.15	128.20
629	6-hydroxy-5-nitro-4-methylcoumarin	105.60	110.37	112.84	117.98
630	7-hydroxy-4-methyl-8-nitro-2H-chromen-2-one	106.00	110.39	112.78	118.00
631	2-naphthalenesulfonylchloride	121.91	121.67	118.88	122.29
632	7-hydroxy-4-methyl-2H-chromen-2-one	99.96	103.47	102.63	103.12
633	5,7-dihydroxy-4-methylcoumarin	106.90	108.86	107.32	107.36
634	naphthalene-1-thiol	109.50	107.91	105.05	95.80
635	naphthalene-1,2-dithiol	118.00	129.42	124.03	104.55
636	4,6-dimethylcoumarin	106.20	110.64	110.45	110.36
637	4,7-dimethylcoumarin	107.60	110.64	110.45	110.37
638	6-methoxy-4-methylcoumarin	109.50	115.96	115.32	114.23
639	7-methoxy-4-methyl-2H-chromen-2-one	110.50	115.96	115.33	114.23
640	methyl n-propyl ketone-2,4-dinitrophenylhydrazone	135.70	131.52	139.97	148.66
641	diphenylsulfane	119.20	119.66	121.77	113.76
642	phenylsulfone	129.00	124.23	121.21	124.33
643	chrysoidine	126.30	123.64	123.99	125.65
644	1-ethoxynaphthalene	119.90	116.04	115.16	114.83
645	methyl n-butyl ketone-2,4-dinitrophenylhydrazone	147.65	142.50	150.93	159.77
646	4,4'-dichloro-2,2'-dinitrobiphenyl	150.00	144.98	150.06	159.11
647	carbazole	119.90	108.04	107.90	110.49
648	diphenyl diazomethane	115.00	118.49	120.18	121.62
649	N,N'-diphenyl urea	127.50	124.86	125.26	127.59
650	p-methoxyazobenzene	118.90	128.68	129.18	129.04
651	N,N-diphenylthiourea	134.90	138.67	137.71	131.47
652	methyldiphenoxyphosphine oxide	153.90	146.92	142.98	143.25
653	acridine	118.80	115.55	115.01	117.27
654	2-phenyl bensofuran	130.50	124.87	123.27	124.46
655	benzyl benzoate	132.20	129.97	129.13	129.78
656	aminoazotoluene	142.20	141.98	142.39	142.78
657	anthraquinone	119.60	125.36	125.12	127.79
658	acetoaminofluorene	141.00	142.29	143.16	144.07
659	9-cyanoanthracene	142.10	128.66	129.16	130.92
660	9-methyl-10-methoxy anthracene	158.10	150.22	148.85	147.38
661	1,4-cycloheptadiene	61.00	69.21	69.03	69.81
662	tri anilino phosphine oxide	201.70	191.51	188.25	190.09
663	aurin	161.40	174.06	171.81	172.22
664	N,N',N-triphenyl urea	176.60	175.97	174.63	176.74
665	anthrazine	245.70	243.88	242.21	245.97
666	anthrone	118.00	124.33	124.46	126.65
667	carbon disulfide	42.20	40.38	40.32	27.29
668	dimethyl furazan	57.27	57.41	59.58	60.11
669	busulphan	118.68	125.43	120.94	123.26
670	phenyl-propylnitrile	78.20	83.65	84.88	85.66
671	tetrahydroquinoline	89.00	91.35	92.31	94.28
672	propyl sulfide	92.10	100.27	100.73	86.23
673	propane-1-thiol	58.50	62.78	59.81	49.37
674	n-octyl mercaptan	115.10	117.72	116.43	104.90
675	thia coumarin	93.60	103.88	104.30	93.08
676	sulfamide	44.40	38.36	35.16	38.18
677	morpholine	55.00	57.13	57.41	58.15
678	nicotine	113.33	108.46	111.82	113.42
679	N-propyl urea	67.40	62.31	63.37	64.14

680	methylol urea	48.30	43.10	43.47	44.35
681	N,N,N',N'-tetramethylurea	75.70	75.87	76.92	75.03
682	nitrosopiperidine	63.40	68.27	72.25	74.08
683	aminomethyldiethyldiazine	114.80	109.83	112.47	112.52
684	2-methylthiophene	66.35	66.49	65.95	58.17
685	acetylthiophene	71.70	77.34	77.96	70.06
686	2-aminothiazole	56.00	55.93	57.12	50.36
687	2-methylthiazole	59.56	61.93	63.37	55.90
688	pyridazine	40.50	43.58	46.28	48.12
689	hexabenz[bc,ef,hi,kl,no,qr]coronene	346.00	352.08	349.45	353.78
690	9-methyl-3,4-benzoacridine	161.10	160.96	160.02	161.59
691	1,2,5,6-dibenzoacridine	186.40	181.85	180.54	183.14
692	2-methylquinoline	99.86	94.83	94.80	95.82
693	4-methylquinoline	94.71	94.56	94.85	96.02
694	5,7,9-trimethyl-1,2-benzoacridine	184.50	188.31	188.94	188.30
695	7-methylquinoline	97.86	94.28	94.61	95.75
696	6-methylquinoline	97.43	94.28	94.66	95.75
697	<i>m</i> -chlorophenol	77.60	73.05	71.01	70.73
698	dimethyl malonate	69.69	71.25	72.23	70.32
699	quinoline	86.00	82.04	82.38	84.34
700	decane	119.50	118.65	120.05	119.55
701	<i>n</i> -heptyl benzene	134.41	132.50	132.64	132.22
702	5-cyclohexylacenaphthene	165.20	171.38	174.49	176.82
703	1,2-dibromoethylene	71.70	75.94	75.54	72.19
704	1,3-dichloro-2-hydroxypropane	80.10	72.71	71.12	71.61
705	tetranitromethane	43.00	55.73	54.45	74.28
706	pyrimidine	43.10	43.70	46.04	47.88
707	thiophene	57.30	55.11	53.98	46.43
708	triazine	37.90	38.89	43.27	45.68
709	1,3,5-trichlorobenzene	106.50	96.82	95.21	92.95
710	phthalic anhydride	66.70	80.87	80.73	83.17
711	glucose	102.60	91.66	89.55	90.16
712	dimethyl sulfate	62.20	61.56	57.05	56.65
713	phenanthrene	127.90	119.53	118.64	120.17
714	2,2-di(chloromethyl)propane	96.90	90.93	89.20	89.94
715	5,11-dibromotetracene	216.00	204.76	205.99	202.63
716	2-naphthalenamine	98.00	92.49	91.67	93.00
717	3,4-bis-(<i>p</i> -hydroxy-phenyl)-2,4-hexadiene	157.00	173.11	170.49	167.73
718	N,N,N',N'-tetraphenylthiourea	229.70	238.32	236.21	229.85
719	anthracenedinitrile	154.60	137.49	139.43	141.57
720	N,N,N',N'-tetraethylthiourea	132.60	135.82	138.41	128.18

TS2. Experimental and calculated diamagnetic susceptibilities of 361 organic compounds (test set)

No	compounds	$-\chi_M(10^{-6}\text{cgs})$			
		Exp.	Cal.1	Cal.2	Cal.3
721	1-nonene	100.10	100.61	100.98	100.51
722	<i>n</i> -hexyl benzene	124.23	121.51	121.44	121.11
723	stilbene	120.00	119.75	118.57	119.12
724	diethyl sebacate	177.00	171.72	174.65	172.72
725	<i>m</i> -iodotoluene	112.30	102.22	102.25	96.34
726	methyldiphenyltriazine	155.10	152.41	154.42	155.78
727	1-phenyl-4-benzoyl-1,3-butadiene	140.80	147.68	146.58	146.98
728	cycloheptene	69.30	74.61	74.59	75.53
729	dimethyl isoxazole	59.70	61.50	62.40	62.43
730	N,N'-dimethylthiourea	64.70	63.99	64.71	56.94
731	thiourea	42.40	39.13	39.24	33.02
732	piperazine	56.80	58.11	58.83	60.09
733	pseudocumene	101.60	90.54	89.65	88.28
734	9-methylanthracene	146.50	132.04	131.29	131.90
735	adonitol	91.30	82.14	78.76	78.86
736	methylfumaric acid	50.98	65.19	65.03	65.12
737	perfluorobutyric anhydride	149.40	150.92	133.05	138.80
738	tryptophan	132.00	117.66	118.20	120.62
739	2-methylcarbanilide	154.00	137.39	137.66	139.28
740	1-nitroso-2-naphthol	83.90	96.90	98.80	100.70
741	<i>o</i> -phenetidine	101.70	89.30	87.88	87.02
742	anthracenenitrile	142.10	128.36	128.93	130.81
743	dichloromethane	46.60	46.52	45.13	46.01
744	camphoric acid	129.00	116.36	119.56	120.71
745	cyclohexanoneoxime-O-methyl ether	82.90	86.76	87.90	86.97
746	methyl- <i>p</i> -hydroxybenzoate	88.70	87.43	85.68	84.67
747	phenyl methyl sulfide	83.20	92.67	91.22	76.75
748	R-aminobutyric acid	62.10	58.89	59.35	60.55
749	isoamyl formate	78.38	75.86	77.38	77.56
750	sorbitol	107.80	97.57	93.48	93.39
751	1,4-butanediol	61.50	58.21	57.22	57.76
752	<i>n</i> -butyraldehyde	46.08	49.23	50.90	51.94
753	dichloroacetic acid	58.20	59.75	58.33	59.77
754	ethyl acetate	54.10	56.40	57.51	56.39
755	fructose	102.60	92.79	90.15	90.45
756	2,3-hexadiene	60.90	64.12	64.47	63.38
757	barbituric acid	53.80	58.51	61.12	64.03
758	cholesterol	284.20	294.00	305.37	303.89
759	triethyl phosphate	125.30	113.06	109.53	106.90
760	diethyl sulfate	86.80	85.09	81.39	81.23
761	1-heptanol	91.70	88.43	88.64	88.65
762	<i>p</i> -chloroanisole	89.10	85.53	83.55	81.88
763	<i>p</i> -chloriodobenzene	99.42	104.40	102.88	98.18
764	<i>o</i> -cresol	72.90	71.15	69.37	69.25
765	2,4-di- <i>tert</i> -butylphenol	155.60	151.42	148.82	146.17
766	<i>p</i> -dinitrobenzene	68.30	65.66	72.62	82.76
767	2-methoxynaphthalene	107.60	103.95	102.89	102.41
768	1-naphthol	95.22	91.77	90.35	91.44
769	1-phenyl-2-methylbutane	113.53	110.90	110.36	110.18
770	durene	101.20	103.04	102.22	100.29
771	tetraphenylethylene	217.40	219.96	217.54	217.17
772	furan	43.09	41.06	40.62	41.04
773	4-methylpyridine	59.80	60.79	61.45	62.08
774	2,5-dimethyl-1-ethylpyrrole	94.61	91.04	91.49	90.26
775	2,5-dimethylfuran	66.37	66.30	65.79	64.45
776	cytosine	55.80	55.23	56.36	58.93
777	thymidine	57.10	64.97	66.65	69.46
778	naphthalene	91.90	86.40	85.76	87.13

779	pyrene	147.90	135.85	135.00	137.02
780	cycloheptane	78.90	80.01	80.03	80.89
781	3-ethylpentane	86.20	86.66	87.84	87.28
782	3-ethylhexane	97.80	97.63	99.14	98.28
783	2,3,4-trimethylpentane	99.80	97.36	97.72	98.25
784	<i>cis</i> -decahydronaphthalene	107.00	109.53	114.13	116.29
785	undecane	131.80	129.64	131.25	130.65
786	perhydroanthracene	146.01	150.03	158.02	160.85
787	hexadecane	187.60	184.57	187.25	186.19
788	4-methylheptane	97.30	97.04	98.56	97.49
789	allene	25.30	27.70	27.48	27.29
790	1,2-butadiene	35.60	40.25	40.14	39.52
791	<i>cis</i> -2-butene	42.60	46.71	46.28	45.42
792	1-pentene	54.60	56.66	56.22	56.09
793	2-methyl-1,3-butadiene	46.00	50.57	49.26	48.50
794	2,3-dimethyl-1,3-butadiene	57.20	62.74	61.10	60.33
795	1-hexene	66.40	67.65	67.34	67.20
796	1,2-octadiene	83.60	84.51	85.01	84.48
797	2-methyl-4-heptene	88.00	91.05	91.08	90.24
798	2,6-dimethyl-2,6,8-nonatriene	108.80	113.04	112.69	109.78
799	1-hexyne	64.50	62.75	63.30	63.55
800	styrene	68.20	70.80	69.12	69.07
801	hydrindene	78.50	85.17	86.12	87.87
802	1,3,5-trimethylbenzene	92.30	90.29	90.17	87.69
803	phenylbutadiene	85.70	87.43	85.66	85.08
804	<i>p</i> -cymene	102.80	101.13	100.09	99.39
805	3,4-dimethyloxadiazole	57.17	61.13	61.81	61.59
806	2-methylnaphthalene	102.70	98.64	98.04	98.54
807	1,6-dimethylnaphthalene	113.30	111.15	110.61	110.22
808	diphenylacetylene	116.00	115.75	115.09	115.87
809	1,2-diphenylethane	127.80	124.37	124.18	124.96
810	9-ethylidene-9H-fluorene	124.80	132.89	132.09	132.30
811	diphenylbutadiene	129.60	137.40	135.71	135.21
812	9-propylanthracene	164.00	154.79	154.44	154.87
813	<i>m</i> -terphenyl	155.50	152.88	151.39	152.12
814	diphenyl octatetraene	164.30	170.64	168.67	167.28
815	1,1-diphenylnonane	206.32	203.37	204.53	204.00
816	indene	83.00	80.08	80.17	81.80
817	diphenyldecapentaene	180.50	187.26	185.17	183.31
818	tetraphenylbutadiene	228.00	237.17	234.01	232.99
819	1-nitropropane	45.00	42.55	49.04	54.61
820	tetraphenyl decapentaene	280.80	287.38	283.86	281.20
821	dibromomethane	65.10	70.32	71.18	72.08
822	diiodomethane	93.10	91.16	91.67	90.03
823	iodomethane	57.20	62.66	65.16	62.33
824	1,2-dibromodiiodoethylene	140.10	141.30	139.52	150.13
825	tetrabromoethylene	114.80	121.60	120.89	129.23
826	chlorotrifluoroethylene	49.10	43.27	43.80	44.85
827	ethylene iodide	104.70	106.56	106.88	101.13
828	<i>cis</i> -1,2-dichloroethylene	51.00	51.48	49.64	49.14
829	1,1-dichloroethane	57.40	56.16	54.53	55.01
830	trichloroethylene	65.80	64.88	62.33	62.07
831	tetraiodoethylene	164.30	159.93	157.34	173.58
832	1-chloropropane	56.00	55.18	54.31	55.01
833	nitrotri(chlormethyl)methane	107.80	100.66	103.23	107.67
834	tetra(chloromethyl)methane	129.00	119.98	120.05	118.87
835	amylene chloride	95.20	84.78	83.63	82.69
836	2,5-dimethyl-2,5-dibromo-3-hexyne	135.60	133.63	133.64	130.31
837	difluoroethanol	41.30	39.19	37.00	37.39
838	glycerol	57.10	51.27	49.27	49.73
839	1,3-butanediol	61.80	58.94	57.82	57.91
840	2-butyne-1,4-diol	50.30	48.41	47.91	47.74

841	dimethyltrichloromethylcarbinol	105.00	95.82	91.52	93.01
842	Cyclopentanol	64.00	62.08	59.61	59.87
843	2-pentanol	69.10	67.19	67.05	66.59
844	1,5-pentanediol	73.50	69.20	68.42	68.87
845	cyclohexenol	64.10	68.42	67.44	68.05
846	2,5-dimethyl-3-hexyne-2,5-diol	103.00	96.44	93.83	91.46
847	dodecyl alcohol	147.70	143.37	144.64	144.18
848	trichloroacetaldehyde	73.00	65.86	64.93	65.99
849	pentanal	57.50	60.22	62.10	63.05
850	furfural	47.20	51.45	52.15	52.98
851	diethyl acetaldehyde	70.71	72.47	74.37	75.07
852	1-acetyl-1-(ethyloxycarbonyl)cyclobutane	103.40	109.54	106.88	105.95
853	2,4-pentanedione	54.90	59.92	62.70	62.39
854	acetonylacetone	62.51	70.90	73.58	73.60
855	hexachlorohexatrione	145.00	154.03	151.01	152.39
856	triquinoyl	71.60	70.18	72.14	76.45
857	fluorenone	99.40	114.19	113.76	116.01
858	oxalic acid	42.90	36.41	36.39	37.62
859	thioacetic acid	38.40	44.16	43.82	36.76
860	trifluoroacetic acid	43.30	42.92	39.18	41.26
861	malonic acid	46.30	46.17	47.04	48.10
862	aspartic acid	64.20	62.93	63.21	64.62
863	chloromaleic acid	67.38	67.36	66.62	66.89
864	fumaric acid	49.10	52.58	52.83	53.54
865	cyclopropanecarboxylic acid	45.33	50.86	44.21	44.54
866	tartric acid	67.50	67.06	65.46	66.51
867	pentanoic acid	66.50	65.93	66.58	67.19
868	valine	74.30	71.88	71.43	72.53
869	methylene succinic acid	57.57	67.19	68.61	70.06
870	methylmaleic acid	57.84	65.19	65.03	65.12
871	cyclopentanecarboxylic acid	73.48	72.83	71.39	71.93
872	octanoic acid	99.50	98.89	100.23	100.51
873	hexadecanoic acid	198.60	186.78	189.83	189.36
874	octadecanoic acid	220.80	208.76	212.23	211.57
875	acepleadiene	135.00	140.45	140.76	142.89
876	tetradecanoic acid	176.00	164.81	167.43	167.15
877	vinyl formate	34.70	36.18	37.41	37.44
878	ethyl iso-thiocyanate	59.00	52.75	55.10	48.20
879	ethyl carbamate	57.00	50.57	51.10	50.94
880	dimethyl oxalate	55.70	61.53	61.60	59.77
881	ethyl iodoacetate	97.60	95.55	97.12	92.69
882	ethyl thiolacetate	62.70	74.77	75.57	63.26
883	methyl butyrate	66.40	67.48	68.17	67.19
884	ethyl lactate	72.60	72.47	72.19	71.33
885	ethyl cyanoacetate	67.30	63.39	66.15	66.24
886	methyl acetoacetate	59.60	65.58	67.39	66.35
887	diethyl oxalate	81.70	85.09	85.62	84.40
888	propyl propionate	77.70	79.26	79.97	79.52
889	triethyl phosphite	104.80	120.35	120.01	116.08
890	ethyl methylacetoacetate	81.90	90.06	91.39	90.77
891	butyl propanoate	89.10	90.25	91.02	90.63
892	propyl butyrate	89.40	90.23	91.05	90.60
893	2-butene-1,4-diyl diacetate(cis)	95.20	98.60	100.07	97.87
894	diethyl succinate	105.00	105.80	107.51	106.08
895	diethyl tartrate	113.40	115.72	114.86	113.29
896	di-iso-propyl oxalate	106.02	107.87	107.77	105.92
897	2-butyne-1,4-diyl diacetate	95.90	94.20	96.34	94.27
898	ethyl propylacetoacetate	105.70	112.59	114.71	113.39
899	ethyl butylmalonate	139.30	141.06	142.54	140.58
900	ethyl-1-methyl-2-oxocyclohexanecarboxylate	112.10	120.35	121.15	121.03
901	ethyl 1-isobutylacetoacetate	121.40	123.35	124.91	123.76
902	ethyl ethylpropylmalonate	152.40	154.72	155.77	152.72

903	ethyl hexylpropiolate	129.90	125.24	126.72	125.55
904	ethyl ethylbutylmalonate	163.30	165.71	166.69	163.82
905	Triethyl citrate	161.90	161.53	162.15	159.03
906	methyloxirane	42.50	41.62	37.56	37.42
907	1,2-epoxybutane	54.80	53.19	49.40	49.17
908	1,1-diethoxyethane	81.40	85.58	85.71	82.78
909	ethyl hydroxylamine	43.00	38.64	39.42	39.67
910	N-nitrosodiethylamine	59.30	63.00	67.64	68.08
911	tri-iso-butylamine	156.80	147.22	149.24	146.39
912	tri-n-hexylamine	221.70	213.84	217.23	215.44
913	carbonyl chloride	47.90	43.21	43.39	43.44
914	dichloroacetyl chloride	69.00	68.76	67.56	69.32
915	iso-butyl chloride	63.90	64.39	64.38	65.32
916	oenanthylidene chloride	116.50	111.77	111.62	111.72
917	oxamide	39.00	38.46	39.30	41.02
918	asparagine	69.50	63.88	64.70	66.31
919	dimethyl oxamide	63.20	62.78	63.76	63.94
920	hexylpropiolamide	103.70	101.89	103.63	103.90
921	succinic anhydride	47.50	51.64	52.38	54.16
922	glycine	39.60	36.92	37.21	38.32
923	leucine	84.90	82.46	82.66	83.02
924	tyrosine	105.30	101.60	100.04	100.65
925	acetoxime-O-methyl-ether	54.87	45.75	47.82	46.16
926	ethyl methyl ketoxime	57.30	56.86	58.37	58.26
927	methyl <i>n</i> -propyl ketone oxime	68.82	67.83	69.85	69.28
928	methyl <i>n</i> -butyl ketone oxime	79.97	78.82	80.81	80.39
929	methyl amyl ketone oxime	91.24	89.80	92.06	91.50
930	octanone oxime	102.70	99.23	102.21	102.30
931	acetophenone oxime	79.90	82.58	82.84	82.55
932	pyridine	48.70	48.55	49.27	50.51
933	2-methylpyridine	60.30	61.33	61.74	62.15
934	3-methylpyridine	59.80	60.82	61.51	62.04
935	2,4-dimethylpyridine	71.30	73.57	74.18	73.66
936	pyrrole	48.60	41.02	41.39	42.70
937	pyrrolidine	54.80	52.58	51.45	52.05
938	2-methylpyrrole	60.10	53.69	53.88	54.43
939	2,3,5-trimethylpyrrole	82.31	78.91	79.10	78.13
940	2,5-dimethyl-3-propyl-pyrrole	106.07	101.66	102.40	101.11
941	3,4-dichloro-1-iodobenzene	118.00	119.08	117.78	112.05
942	<i>p</i> -bromotoluene	88.70	91.52	90.94	88.92
943	1-iodo-2-phenylacetylene	110.10	104.10	102.94	97.03
944	1-bromonaphthalene	123.60	112.43	112.69	111.66
945	4,4'-dibromobiphenyl	151.30	154.66	154.51	151.41
946	chloromethylstilbene	144.80	146.53	145.09	144.90
947	<i>p</i> -nitrosotoluene	70.40	70.56	73.14	73.98
948	<i>o</i> -dinitrobenzene	65.98	66.19	72.71	82.86
949	<i>o</i> -nitrotoluene	72.20	72.24	75.01	79.73
950	phthalamide	91.30	88.41	87.85	88.99
951	benzylideneamino-1-hydroxyethane	91.00	93.80	92.88	92.58
952	<i>m</i> -chloroaniline	76.60	74.07	72.52	72.44
953	<i>p</i> -chloroaniline	76.70	74.07	72.29	72.47
954	<i>o</i> -chloroaniline	79.50	74.35	72.47	72.81
955	<i>m</i> -phenylenediamine	70.40	65.75	64.51	65.14
956	N-methylaniline	74.10	72.08	71.35	71.06
957	phenyl propioplamide	83.30	94.57	94.46	94.76
958	mannose	102.90	91.66	89.55	90.16
959	dibenz[a,h]anthracene	193.00	185.50	183.99	185.91
960	N-2-naphthylacetamide	117.80	115.52	116.04	116.57
961	<i>m</i> -nitro carbanilide	148.10	136.96	145.23	156.90
962	chorodifluoromethylbenzol	87.20	85.35	82.30	82.92
963	1-chloro-2-nitrobenzene	75.50	74.42	76.64	81.52
964	3-nitrocarbanilide	148.10	130.91	135.25	142.24

965	2-naphthol	96.80	91.46	90.18	91.30
966	2,6-di- <i>tert</i> -bntyl-4-methyl phenol	165.30	163.98	161.55	157.70
967	<i>p</i> -nitrosophenol	60.70	63.39	65.37	66.72
968	Cyclododecene	127.00	129.55	131.72	132.80
969	phloroglucinol	73.40	68.77	66.11	65.99
970	<i>m</i> -cresol	72.20	70.87	69.38	68.98
971	<i>p</i> -cresol	72.40	70.86	69.21	69.01
972	carvacrol	109.10	106.49	104.68	103.92
973	2-nitroso-1-naphthol	82.70	96.88	98.77	100.70
974	1-(<i>p</i> -chloro phenylazo)-2-naphthol	161.40	164.12	163.07	164.18
975	1,5-cyclooctadiene	71.50	80.20	80.46	81.33
976	1-(<i>o</i> -tolylazo)-2-naphthol	148.70	162.25	161.69	162.66
977	1-(<i>p</i> -tolylazo)-2-naphthol	157.60	161.94	161.46	162.42
978	saligenin(salicylalcohol)	76.90	74.69	72.31	72.45
979	estradiol	186.60	188.70	194.14	195.47
980	anisole	72.20	71.11	69.70	68.54
981	<i>o</i> -cresylmethyl ether	81.94	83.65	82.30	80.33
982	<i>m</i> -cresylmethyl ether	77.91	83.35	82.08	80.09
983	<i>p</i> -phenetidine	96.80	88.98	87.72	86.87
984	cinnamic aldehyde	74.80	80.07	80.46	80.93
985	citral	98.90	105.68	107.34	105.63
986	salicylic acid	75.00	75.18	73.19	73.73
987	phthalic acid	83.60	86.35	84.84	85.58
988	<i>p</i> -toluic acid	82.40	82.04	80.76	80.86
989	phenyl-propionic acid	81.00	82.40	81.63	81.97
990	(E)-2-(3-phenylallylidene)malonic acid	105.40	119.36	117.53	117.35
991	biphenyl-4-yl(phenyl)methanone	158.00	164.05	162.74	163.90
992	tropolone	61.00	69.75	68.78	69.81
993	propiophenone	83.73	88.50	88.29	88.53
994	ethylacetophenone	95.50	99.47	99.36	99.60
995	trimethyl acetophenone	108.20	110.89	109.69	109.04
996	valerylphenylacetylene	119.00	123.02	123.26	123.33
997	dimethylallylacetophenone	122.40	126.88	125.61	124.51
998	methylethylallylacetophenone	133.30	138.95	137.87	136.88
999	flavone	120.00	135.98	134.76	136.26
1,000	ethyl diallyl acetophenone	147.40	154.91	153.89	152.05
1,001	7,7'-bis(cycloheptatrienyl)	119.00	122.31	123.13	124.08
1,002	salol	123.20	125.15	123.14	123.70
1,003	4-aminostilbene	122.50	125.84	124.41	125.00
1,004	triphenyl phosphite	183.70	197.08	194.77	193.11
1,005	methyl benzoate	81.60	82.36	81.21	80.35
1,006	methyl salicylate	86.60	87.74	85.85	84.80
1,007	ethyl benzoate	93.80	94.15	93.19	92.66
1,008	methyl- <i>o</i> -methoxybenzoate	95.60	100.23	98.65	95.89
1,009	dimethyl terephthalate	101.60	111.16	109.91	107.59
1,010	<i>n</i> -propyl benzoate	105.00	105.11	104.04	103.77
1,011	ethyl amylpropionate	112.70	114.25	115.52	114.45
1,012	ethyl dibromocinnamate	174.50	162.85	163.03	158.98
1,013	ethyl benzoylacetate	115.30	115.02	115.44	115.03
1,014	ethyl phenylmalonate	142.20	144.53	144.31	142.40
1,015	benzyl butyrate	116.30	115.09	114.73	114.32
1,016	ethyl benzylmalonate	154.50	154.91	155.12	153.19
1,017	pentyl benzoate	128.50	127.09	126.36	125.98
1,018	benzyl 2-phenylacetate	143.70	139.93	139.87	140.33
1,019	2-butyne-1,4-dibenzoate	169.00	169.57	169.05	169.48
1,020	galactose	103.00	91.66	89.55	90.16
1,021	benzaldoxime	69.80	69.50	70.32	70.81
1,022	N-methyl-N'-phenylurea	93.35	88.58	88.62	89.14
1,023	benzeneacetonitrile	76.90	72.68	73.67	74.52
1,024	indole	85.00	74.38	74.97	77.39
1,025	7-hydroxy-2H-chromen-2-one	88.22	90.95	90.07	91.47
1,026	ethyl methyl ketone-2,4-dinitrophenylhydrazone	124.11	120.55	128.50	137.64

1,027	camphor	103.00	112.02	115.45	117.45
1,028	7-hydroxy-4-methyl-6-nitro-2H-chromen-2-one	105.50	109.95	112.67	117.91
1,029	6-hydroxy-4-methyl-2H-chromen-2-one	98.69	103.47	102.61	103.12
1,030	7,8-dihydroxy-4-methyl-2H-chromen-2-one	105.10	109.19	107.22	107.54
1,031	1-Methoxynaphthalene	107.00	104.26	103.15	102.53
1,032	5-hydroxy-4,7-dimethylcoumarin	113.50	116.03	115.21	114.59
1,033	diethyl ketone-2,4-dinitrophenylhydrazone	135.16	132.38	140.77	149.67
1,034	N,N'-diethyl-N'-phenylurea	126.40	125.04	125.02	124.79
1,035	azobenzene	106.80	111.13	112.07	113.76
1,036	aminoazobenzene	118.30	117.55	118.07	119.80
1,037	2-ethoxynaphthalene	119.20	115.73	114.96	114.71
1,038	2,4'-dinitrobiphenyl	116.50	115.72	122.36	132.70
1,039	N,N-diphenyl urea	126.30	127.13	126.01	127.55
1,040	N,N'-diphenylthiourea	136.50	138.28	138.09	131.48
1,041	methyl amyl ketone-2,4-dinitrophenylhydrazone	156.84	153.49	162.19	170.88
1,042	diphenyldihydropyridazine	129.90	139.13	140.33	143.76
1,043	<i>m</i> -azotoluene	127.80	135.61	136.66	136.55
1,044	azotoluene	135.10	135.60	136.36	136.61
1,045	methyl n-hexyl ketone-2,4-dinitrophenylhydrazone	171.73	164.48	173.39	181.98
1,046	1,3,5-cycloheptatriene	59.80	63.91	63.66	64.34
1,047	N,N'-dimethyl-N,N'-diphenylurea	148.90	149.93	149.80	150.72
1,048	phenanthrenonitrile	139.00	128.65	129.19	130.95
1,049	phenyl ethyl sulfide	94.40	101.74	100.70	87.79
1,050	arabinose	85.70	76.23	74.82	75.63
1,051	phenothiazine	114.80	124.45	127.53	121.13
1,052	anethole	96.00	100.69	99.13	96.57
1,053	cyanamide	24.80	18.61	21.11	22.31
1,054	isoquinoline	83.90	81.41	82.24	84.28
1,055	1,3-cycloheptadiene	61.00	69.26	69.16	70.05
1,056	triethylphosphine oxide	91.60	95.47	95.46	97.41
1,057	dicetyl sulfide	401.70	385.93	392.37	374.99
1,058	ethanethiol	47.00	51.61	48.79	38.26
1,059	1-butanethiol	70.20	73.77	71.81	60.48
1,060	thiophosgene	50.60	55.58	53.90	47.26
1,061	N,N-dimethylthiourea	64.20	63.28	63.36	56.28
1,062	thiobarbituric acid	72.90	70.29	72.86	67.91
1,063	N-allylthiourea	69.00	67.14	67.06	60.09
1,064	cyanogen chloride	32.40	27.52	29.03	29.43
1,065	N,N-dimethyl urea	55.10	51.50	52.09	52.20
1,066	N,N'-dimethyl urea	56.30	52.21	53.42	52.99
1,067	urea	33.50	27.16	28.04	29.20
1,068	N-methyl urea	44.60	39.68	40.61	41.11
1,069	N-ethyl urea	55.50	51.34	52.48	53.03
1,070	N,N'-diethylurea	74.10	75.53	76.99	76.85
1,071	N,N,N',N'-tetraethylurea	122.40	124.22	125.94	124.10
1,072	piperidine	64.20	63.57	63.47	64.47
1,073	cyanogen	21.60	12.52	14.69	15.85
1,074	thiazole	50.55	50.04	51.32	44.20
1,075	5,5-dimethylcyclopentadiene	67.50	70.54	69.25	68.88
1,076	cyclopentene	49.50	52.64	50.84	51.20
1,077	acenaphthanthracene	184.00	176.91	175.94	178.72
1,078	2,4-dimethylquinoline	108.54	107.35	107.55	107.46
1,079	5,7,8,9-tetramethyl-3,4-benzoacridine	196.30	199.06	198.19	197.17
1,080	8-methylquinoline	96.57	94.60	94.90	95.97
1,081	5,7,9-trimethyl-3,4-benzoacridine	183.70	186.28	185.37	185.11

TS3. Values of the standard error of estimate for various values of the parameters a , b and y

No	a	y	b	s	No	a	y	b	s	No	a	y	b	s
1	1.00	0.46	1.0	5.3903	132	1.05	0.42	2.5	5.3413	263	1.10	0.32	1.0	5.4492
2	1.00	0.46	1.1	5.3861	133	1.05	0.42	3.0	5.4088	264	1.10	0.32	1.5	5.3920
3	1.00	0.46	1.2	5.3840	134	1.05	0.42	3.5	5.4635	265	1.10	0.32	2.0	5.3598
4	1.00	0.46	1.3	5.3839	135	1.05	0.42	4.0	5.5456	266	1.10	0.32	2.5	5.3410
5	1.00	0.46	1.4	5.3859	136	1.05	0.40	1.0	5.3513	267	1.10	0.32	3.0	5.3156
6	1.00	0.46	1.5	5.3899	137	1.05	0.40	1.5	5.3012	268	1.10	0.32	3.5	5.3042
7	1.00	0.46	1.6	5.3940	138	1.05	0.40	1.9	5.2818	269	1.10	0.32	3.6	5.3034
8	1.00	0.46	2.0	5.4036	139	1.05	0.40	2.0	5.2785	270	1.10	0.32	3.7	5.3019
9	1.00	0.46	2.5	5.4187	140	1.05	0.40	2.1	5.2763	271	1.10	0.32	3.8	5.3006
10	1.00	0.46	3.0	5.4987	141	1.05	0.40	2.2	5.2752	272	1.10	0.32	3.9	5.2999
11	1.00	0.46	3.5	5.6611	142	1.05	0.40	2.3	5.2753	273	1.10	0.32	4.0	5.2995
12	1.00	0.46	4.0	5.8075	143	1.05	0.40	2.4	5.2764	274	1.10	0.32	4.1	5.2997
13	1.00	0.46	4.5	5.9664	144	1.05	0.40	2.5	5.2787	275	1.10	0.32	4.2	5.3002
14	1.00	0.46	5.0	6.1686	145	1.05	0.40	2.6	5.2821	276	1.10	0.32	4.3	5.3012
15	1.00	0.44	1.0	5.3839	146	1.05	0.40	3.0	5.3067	277	1.15	0.46	0.4	5.8870
16	1.00	0.44	1.4	5.3522	147	1.05	0.40	3.5	5.3628	278	1.15	0.46	0.5	5.8796
17	1.00	0.44	1.5	5.3485	148	1.05	0.40	4.0	5.4480	279	1.15	0.46	0.6	5.8742
18	1.00	0.44	1.6	5.3465	149	1.05	0.38	1.0	5.3962	280	1.15	0.46	0.7	5.8709
19	1.00	0.44	1.7	5.3461	150	1.05	0.38	1.5	5.3277	281	1.15	0.46	0.8	5.8694
20	1.00	0.44	1.8	5.3474	151	1.05	0.38	2.0	5.2879	282	1.15	0.46	0.9	5.8699
21	1.00	0.44	1.9	5.3504	152	1.05	0.38	2.5	5.2728	283	1.15	0.46	1.0	5.8723
22	1.00	0.44	2.0	5.3551	153	1.05	0.38	2.6	5.2709	284	1.15	0.46	1.5	5.9119
23	1.00	0.44	2.5	5.3892	154	1.05	0.38	2.7	5.2698	285	1.15	0.46	2.0	5.9966
24	1.00	0.44	3.0	5.4196	155	1.05	0.38	2.8	5.2697	286	1.15	0.46	2.5	6.1266
25	1.00	0.44	3.5	5.4764	156	1.05	0.38	2.9	5.2704	287	1.15	0.46	3.0	6.3030
26	1.00	0.44	4.0	5.5948	157	1.05	0.38	3.0	5.2720	288	1.15	0.46	4.0	6.8033
27	1.00	0.44	4.5	5.7845	158	1.05	0.38	3.1	5.2745	289	1.15	0.44	0.7	5.7595
28	1.00	0.44	5.0	5.9325	159	1.05	0.38	3.5	5.2931	290	1.15	0.44	0.8	5.7568
29	1.00	0.42	1.0	5.4166	160	1.05	0.38	4.0	5.3365	291	1.15	0.44	0.9	5.7519
30	1.00	0.42	1.5	5.3555	161	1.05	0.36	1.0	5.4496	292	1.15	0.44	1.0	5.7486
31	1.00	0.42	1.9	5.3319	162	1.05	0.36	1.5	5.3915	293	1.15	0.44	1.1	5.7470
32	1.00	0.42	2.0	5.3294	163	1.05	0.36	2.0	5.3360	294	1.15	0.44	1.2	5.7470
33	1.00	0.42	2.1	5.3282	164	1.05	0.36	2.5	5.3023	295	1.15	0.44	1.3	5.7486
34	1.00	0.42	2.2	5.3284	165	1.05	0.36	2.8	5.2917	296	1.15	0.44	1.4	5.7517
35	1.00	0.42	2.3	5.3299	166	1.05	0.36	2.9	5.2897	297	1.15	0.44	1.5	5.7563
36	1.00	0.42	2.4	5.3328	167	1.05	0.36	3.0	5.2884	298	1.15	0.44	2.0	5.8024
37	1.00	0.42	2.5	5.3371	168	1.05	0.36	3.1	5.2879	299	1.15	0.44	2.5	5.8859
38	1.00	0.42	3.0	5.3690	169	1.05	0.36	3.2	5.2881	300	1.15	0.44	3.0	6.0076
39	1.00	0.42	3.5	5.4293	170	1.05	0.36	3.3	5.2888	301	1.15	0.44	3.5	6.1690
40	1.00	0.42	4.0	5.4869	171	1.05	0.36	3.5	5.2894	302	1.15	0.44	4.0	6.3724
41	1.00	0.42	4.5	5.5625	172	1.05	0.36	4.0	5.3030	303	1.15	0.42	0.8	5.6054
42	1.00	0.42	5.0	5.6991	173	1.05	0.34	1.0	5.4844	304	1.15	0.42	0.9	5.6014
43	1.00	0.40	1.0	5.4815	174	1.05	0.34	1.5	5.4302	305	1.15	0.42	1.0	5.5995
44	1.00	0.40	1.5	5.4027	175	1.05	0.34	2.0	5.4009	306	1.15	0.42	1.1	5.5994
45	1.00	0.40	2.0	5.3534	176	1.05	0.34	2.5	5.3738	307	1.15	0.42	1.2	5.6013
46	1.00	0.40	2.4	5.3337	177	1.05	0.34	3.0	5.3439	308	1.15	0.42	1.3	5.6051
47	1.00	0.40	2.5	5.3315	178	1.05	0.34	3.5	5.3289	309	1.15	0.42	1.5	5.6181
48	1.00	0.40	2.6	5.3303	179	1.05	0.34	3.6	5.3276	310	1.15	0.42	2.0	5.6570
49	1.00	0.40	2.7	5.3302	180	1.05	0.34	3.7	5.3268	311	1.15	0.42	2.5	5.7135
50	1.00	0.40	2.8	5.3312	181	1.05	0.34	3.8	5.3266	312	1.15	0.42	3.0	5.7910
51	1.00	0.40	2.9	5.3333	182	1.05	0.34	3.9	5.3270	313	1.15	0.42	3.5	5.9001
52	1.00	0.40	3.0	5.3364	183	1.05	0.34	4.0	5.3279	314	1.15	0.42	4.0	6.0426
53	1.00	0.40	3.5	5.3649	184	1.05	0.34	4.1	5.3294	315	1.15	0.40	1.0	5.4898
54	1.00	0.40	4.0	5.4127	185	1.10	0.46	1.0	5.6325	316	1.15	0.40	1.3	5.4736
55	1.00	0.40	4.5	5.4877	186	1.10	0.46	1.1	5.6310	317	1.15	0.40	1.4	5.4715
56	1.00	0.40	5.0	5.5740	187	1.10	0.46	1.2	5.6233	318	1.15	0.40	1.5	5.4710
57	1.00	0.38	1.5	5.4708	188	1.10	0.46	1.3	5.6200	319	1.15	0.40	1.6	5.4721
58	1.00	0.38	2.0	5.4176	189	1.10	0.46	1.4	5.6212	320	1.15	0.40	1.7	5.4747
59	1.00	0.38	2.5	5.3755	190	1.10	0.46	1.5	5.6267	321	1.15	0.40	2.0	5.4917
60	1.00	0.38	2.9	5.3572	191	1.10	0.46	2.0	5.6965	322	1.15	0.40	2.5	5.5473

61	1.00	0.38	3.0	5.3547	192	1.10	0.46	2.5	5.7882	323	1.15	0.40	3.0	5.6100
62	1.00	0.38	3.1	5.3531	193	1.10	0.46	3.0	5.9214	324	1.15	0.40	3.5	5.7043
63	1.00	0.38	3.2	5.3523	194	1.10	0.46	3.5	6.0982	325	1.15	0.40	4.0	5.8095
64	1.00	0.38	3.3	5.3523	195	1.10	0.46	4.0	6.3218	326	1.15	0.38	1.0	5.4241
65	1.00	0.38	3.4	5.3532	196	1.10	0.44	0.7	5.5071	327	1.15	0.38	1.5	5.3855
66	1.00	0.38	3.5	5.3549	197	1.10	0.44	0.8	5.5029	328	1.15	0.38	1.7	5.3792
67	1.00	0.38	4.0	5.3765	198	1.10	0.44	0.9	5.5008	329	1.15	0.38	1.8	5.3779
68	1.00	0.38	4.5	5.4142	199	1.10	0.44	1.0	5.5006	330	1.15	0.38	1.9	5.3768
69	1.00	0.38	5.0	5.4707	200	1.10	0.44	1.1	5.5024	331	1.15	0.38	2.0	5.3768
70	1.00	0.36	1.0	5.5812	201	1.10	0.44	1.5	5.5276	332	1.15	0.38	2.1	5.3780
71	1.00	0.36	1.5	5.5146	202	1.10	0.44	2.0	5.5535	333	1.15	0.38	2.2	5.3805
72	1.00	0.36	2.0	5.4747	203	1.10	0.44	2.5	5.6062	334	1.15	0.38	2.5	5.3952
73	1.00	0.36	2.5	5.4538	204	1.10	0.44	3.0	5.7224	335	1.15	0.38	3.0	5.4434
74	1.00	0.36	3.0	5.4211	205	1.10	0.44	3.5	5.8439	336	1.15	0.38	3.5	5.5177
75	1.00	0.36	3.5	5.3998	206	1.10	0.44	4.0	6.0028	337	1.15	0.38	4.0	5.5941
76	1.00	0.36	3.7	5.3957	207	1.10	0.42	1.0	5.4069	338	1.15	0.36	1.0	5.4003
77	1.00	0.36	3.8	5.3947	208	1.10	0.42	1.1	5.4019	339	1.15	0.36	1.5	5.3423
78	1.00	0.36	3.9	5.3943	209	1.10	0.42	1.2	5.3986	340	1.15	0.36	2.0	5.3126
79	1.00	0.36	4.0	5.3945	210	1.10	0.42	1.3	5.3969	341	1.15	0.36	2.1	5.3097
80	1.00	0.36	4.2	5.3954	211	1.10	0.42	1.4	5.3968	342	1.15	0.36	2.2	5.3078
81	1.00	0.36	4.4	5.3991	212	1.10	0.42	1.5	5.3983	343	1.15	0.36	2.3	5.3069
82	1.00	0.36	4.5	5.4056	213	1.10	0.42	2.0	5.4294	344	1.15	0.36	2.4	5.3069
83	1.00	0.36	5.0	5.4343	214	1.10	0.42	2.5	5.4885	345	1.15	0.36	2.5	5.3078
84	1.00	0.36	5.5	5.4766	215	1.10	0.42	3.0	5.5406	346	1.15	0.36	2.6	5.3097
85	1.00	0.34	1.0	5.6377	216	1.10	0.42	3.5	5.6317	347	1.15	0.36	3.0	5.3259
86	1.00	0.34	1.5	5.5773	217	1.10	0.42	4.0	5.7779	348	1.15	0.36	3.5	5.3657
87	1.00	0.34	2.0	5.5272	218	1.10	0.40	1.0	5.3617	349	1.15	0.36	4.0	5.4271
88	1.00	0.34	2.5	5.4957	219	1.10	0.40	1.5	5.3253	350	1.15	0.34	1.0	5.4147
89	1.00	0.34	3.0	5.4800	220	1.10	0.40	1.6	5.3221	351	1.15	0.34	1.5	5.3453
90	1.00	0.34	3.5	5.4782	221	1.10	0.40	1.7	5.3203	352	1.15	0.34	2.0	5.2993
91	1.00	0.34	4.0	5.4674	222	1.10	0.40	1.8	5.3198	353	1.15	0.34	2.5	5.2750
92	1.00	0.34	4.5	5.4527	223	1.10	0.40	1.9	5.3206	354	1.15	0.34	2.6	5.2725
93	1.00	0.34	4.7	5.4468	224	1.10	0.40	2.0	5.3227	355	1.15	0.34	2.7	5.2708
94	1.00	0.34	4.9	5.4437	225	1.10	0.40	2.5	5.3519	356	1.15	0.34	2.8	5.2698
95	1.00	0.34	5.0	5.4432	226	1.10	0.40	3.0	5.4121	357	1.15	0.34	2.9	5.2695
96	1.00	0.34	5.1	5.4434	227	1.10	0.40	3.5	5.4922	358	1.15	0.34	3.0	5.2700
97	1.00	0.34	5.3	5.4459	228	1.10	0.40	4.0	5.5680	359	1.15	0.34	3.1	5.2711
98	1.00	0.34	5.5	5.4513	229	1.10	0.38	1.0	5.3591	360	1.15	0.34	3.5	5.2826
99	1.05	0.46	0.5	5.4579	230	1.10	0.38	1.5	5.3023	361	1.15	0.34	4.0	5.3119
100	1.05	0.46	0.6	5.4492	231	1.10	0.38	2.0	5.2748	362	1.15	0.32	1.0	5.4509
101	1.05	0.46	0.7	5.4426	232	1.10	0.38	2.1	5.2725	363	1.15	0.32	1.5	5.3786
102	1.05	0.46	0.8	5.4382	233	1.10	0.38	2.2	5.2713	364	1.15	0.32	2.0	5.3308
103	1.05	0.46	0.9	5.4358	234	1.10	0.38	2.3	5.2712	365	1.15	0.32	2.5	5.2939
104	1.05	0.46	1.0	5.4356	235	1.10	0.38	2.4	5.2720	366	1.15	0.32	3.0	5.2730
105	1.05	0.46	1.1	5.4374	236	1.10	0.38	2.5	5.2739	367	1.15	0.32	3.1	5.2706
106	1.05	0.46	1.2	5.4413	237	1.10	0.38	3.0	5.2981	368	1.15	0.32	3.2	5.2688
107	1.05	0.46	1.5	5.4652	238	1.10	0.38	3.5	5.3471	369	1.15	0.32	3.3	5.2676
108	1.05	0.46	2.0	5.4552	239	1.10	0.38	4.0	5.3693	370	1.15	0.32	3.4	5.2669
109	1.05	0.46	2.5	5.5426	240	1.10	0.36	1.0	5.3804	371	1.15	0.32	3.5	5.2668
110	1.05	0.46	3.0	5.6841	241	1.10	0.36	1.5	5.3183	372	1.15	0.32	3.6	5.2672
111	1.05	0.46	3.5	5.8136	242	1.10	0.36	2.0	5.2772	373	1.15	0.32	3.7	5.2681
112	1.05	0.46	4.0	5.9844	243	1.10	0.36	2.5	5.2547	374	1.15	0.32	4.0	5.2739
113	1.05	0.44	1.0	5.3691	244	1.10	0.36	2.6	5.2528	375	1.15	0.30	1.0	5.4672
114	1.05	0.44	1.1	5.3639	245	1.10	0.36	2.7	5.2516	376	1.15	0.30	1.5	5.4040
115	1.05	0.44	1.2	5.3604	246	1.10	0.36	2.8	5.2513	377	1.15	0.30	2.0	5.3662
116	1.05	0.44	1.3	5.3587	247	1.10	0.36	2.9	5.2517	378	1.15	0.30	2.5	5.3462
117	1.05	0.44	1.4	5.3588	248	1.10	0.36	3.0	5.2530	379	1.15	0.30	3.0	5.3224
118	1.05	0.44	1.5	5.3605	249	1.10	0.36	3.1	5.2550	380	1.15	0.30	3.1	5.3193
119	1.05	0.44	2.0	5.3945	250	1.10	0.36	3.5	5.2707	381	1.15	0.30	3.2	5.3162
120	1.05	0.44	2.5	5.4331	251	1.10	0.36	4.0	5.3078	382	1.15	0.30	3.3	5.3125
121	1.05	0.44	3.0	5.4821	252	1.10	0.34	1.0	5.4268	383	1.15	0.30	3.4	5.3092
122	1.05	0.44	3.5	5.6150	253	1.10	0.34	1.5	5.3624	384	1.15	0.30	3.5	5.3064

123	1.05	0.44	4.0	5.7722	254	1.10	0.34	2.0	5.3126	385	1.15	0.30	3.6	5.3040
124	1.05	0.42	1.0	5.3436	255	1.10	0.34	2.5	5.2839	386	1.15	0.30	3.9	5.2995
125	1.05	0.42	1.5	5.3102	256	1.10	0.34	3.0	5.2651	387	1.15	0.30	4.0	5.2989
126	1.05	0.42	1.6	5.3070	257	1.10	0.34	3.1	5.2631	388	1.15	0.30	4.1	5.2986
127	1.05	0.42	1.7	5.3053	258	1.10	0.34	3.2	5.2617	389	1.15	0.30	4.2	5.2987
128	1.05	0.42	1.8	5.3049	259	1.10	0.34	3.3	5.2609	390	1.15	0.30	4.3	5.2992
129	1.05	0.42	1.9	5.3060	260	1.10	0.34	3.4	5.2608	391	1.15	0.30	4.5	5.3014
130	1.05	0.42	2.0	5.3084	261	1.10	0.34	3.5	5.2612	392	1.15	0.30	5.0	5.3134
131	1.05	0.42	2.1	5.3123	262	1.10	0.34	4.0	5.2723					