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Research article

Thermodynamic explanation and criterion for the exhibition of melting inability in molecular species

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Supplementary

Table S1. $\Delta H_{melting}$ [1] and ΔH_{max} values for various hydrocarbons.

	Substance	$\Delta H_{melting}, kJ/mol$	$\Delta H_{max}, kJ/mol$
1	methane	0.9	4
2	ethane	2.8	6
3	propane	3.5	8
4	butane	4.7	10
5	isobutane	4.5	10
6	cyclobutane	1.1	8
7	pentane	8.4	12
8	isopentane	5.1	12
9	cyclopentane	0.6	10
10	hexane	13.1	14
11	isohexane	6.3	14
12	cyclohexane	2.7	12
13	octane	21.8	18
14	dodecane	36.8	26
15	eicosane	69.8	42
16	cyclooctane	2.4	16
17	benzene	9.9	16
18	toluene	6.6	18
19	naphthalene	19.1	28
20	anthracene	29.4	40
21	ethene	3.4	4
22	propene	3.0	6
23	1-pentene	5.8	10
24	1-hexene	9.3	12
25	1-octene	15.3	16

Table S2. $\Delta H_{melting}$ [1] and ΔH_{max} values for various ethers.

	Substance	$\Delta H_{melting}, kJ/mol$	$\Delta H_{max}, kJ/mol$
1	dimethyl ether	4.9	16
2	diethyl ether	7.2	20
3	di-n-propyl ether	9.5	24
4	methyl phenyl ether (anisole)	12.9	28
5	diphenyl ether	17.2	40
6	Tetrahydrofuran (1-oxacyclopentane)	8.5	18
7	1,4- dioxane (1,4-dioxacyclohexane)	12.8	28

Table S3. $\Delta H_{melting}$ [1] and ΔH_{max} values for various ketones.

	Substance	$\Delta H_{melting}, kJ/mol$	$\Delta H_{max}, kJ/mol$
1	acetone	5.7	16
2	2-butanone	8.4	18
3	2-pentanone	10.6	20
4	2-hexanone	14.9	22
5	2-octanone	24.4	26
6	methyl phenyl ketone (acetophenone)	16.7	28
7	diphenyl ketone (benzophenone)	18.5	40

Table S4. $\Delta H_{melting}$ [1] and ΔH_{max} values for various acids.

	Substance	$\Delta H_{melting}, kJ/mol$	$\Delta H_{max}, kJ/mol$
1	methanoic acid	12.7	126
2	ethanoic acid	11.7	128
3	propanoic acid	10.7	130
4	butanoic acid	11.1	132
5	benzoic acid	17.3	140

Table S5. $\Delta H_{melting}$[1] and ΔH_{max} values for various alcohols.

	Substance	$\Delta H_{melting}, kJ/mol$	$\Delta H_{max}, kJ/mol$
1	methanol	3.2	78
2	ethanol	4.6	80
3	1-propanol	5.4	82
4	1-butanol	9.3	84
5	1-pentanol	10.5	86
6	1-hexanol	15.4	88
7	1-octanol	25.2	92
8	1-dodecanol	40.3	100
9	2-propanol	5.4	82
10	2-butanol	6.0	84
11	isobutanol	6.3	84
12	phenol	11.5	90
13	1-naphthalenol	23.3	102
14	1,2 ethanediol	10.0	154
15	1,3 propanediol	11.4	156
16	1,5 pentanediol	15.7	160
17	1,4-benzenediol (hydroquinone)	27.1	164
18	1,2,3-propanetriol (glycerin)	18.3	230

Table S6. AMI values for the substances presented in Table S1–Table S5.

	Substance	$AMI, kJoule/mol$
1	methane	–98
2	ethane	–98
3	Propane	–97
4	butane	–96
5	isobutane	–96
6	cyclobutane	–97
7	pentane	–95
8	isopentane	–95
9	cyclopentane	–96
10	hexane	–94
11	isohexane	–94
12	cyclohexane	–95
13	octane	–93
14	dodecane	–89
15	eicosane	–83
16	cyclooctane	–94
17	benzene	–94
18	toluene	–93
19	naphthalene	–89
20	anthracene	–84
21	ethene	–98
22	propene	–98
23	1-pentene	–96
24	1-hexene	–95
25	1-octene	–94
26	dimethyl ether	–94
27	diethyl ether	–92
28	di-n-propyl ether	–90
29	methyl phenyl ether (anisole)	–89
30	diphenyl ether	–84
31	Tetrahydrofuran (1-Oxacyclopentane)	–93
32	1,4-dioxane (1,4-Dioxacyclohexane)	–89
33	acetone	–94
34	2-butanone	–93
35	2-pentanone	–92
36	2-hexanone	–91
37	2-octanone	–89

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	Substance	$AMI, kJoule/mol$
38	methyl phenyl ketone (Acetophenone)	–89
39	diphenyl ketone (Benzophenone)	–84
40	methanoic acid	–49
41	ethanoic acid	–48
42	propanoic acid	–47
43	butanoic acid	–46
44	benzoic acid	–43
45	methanol	–68
46	ethanol	–68
47	1-propanol	–67
48	1-butanol	–66
49	1-pentanol	–65
50	1-hexanol	–64
51	1-octanol	–63
52	1-dodecanol	–59
53	2-propanol	–67
54	2-butanol	–66
55	isobutanol	–66
56	phenol	–63
57	1-Naphthalenol	–59
58	1,2 ethanediol	–37
59	1,3 propanediol	–37
60	1,5 pentanediol	–35
61	1,4-benzenediol (hydroquinone)	–33
62	1,2,3-propanetriol (glycerin)	–7

Table S7. Parameters used for the calculation of $\Delta H_{max}$of the 62 substances presented in Table S6.

	Low polarity groups	Polar groups		Hydrogen bonded groups					Aromatic rings
Number of sites for hydrogen bonded groups (s_{hb})	1	1	1	3	4	5	2	3	1
Representative groups	C-H	C-O, C_3-N, C-F	C=O	OH	NH_2	COOH	C-O, C=O, C-N	NH	aromatic rings
Substance	N_{lp}	N_p	N_p	N_{hb}	N_{hb}	N_{hb}	N_{hb}	N_{hb}	N_{ar}
methane	4								
ethane	6								
Propane	8								
butane	10								

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	Low polarity groups	Polar groups		Hydrogen bonded groups					Aromatic rings
isobutane	10								
cyclobutane	8								
pentane	12								
Representative groups	C-H	C-O, C_3-N, C-F	C=O	OH	NH_2	COOH	C-O, C=O, C-N	NH	aromatic rings
Substance	N_{lp}	N_p	N_p	N_{hb}	N_{hb}	N_{hb}	N_{hb}	N_{hb}	N_{ar}
isopentane	12								
cyclopentane	10								
hexane	14								
isohexane	14								
cyclohexane	12								
octane	18								
dodecane	26								
eicosane	42								
cyclooctane	16								
benzene	6								1
toluene	8								1
naphthalene	8								2
anthracene	10								3
ethene	4								
propene	6								
1-pentene	10								
1-hexene	12								
1-octene	16								
dimethyl ether	6	1							
diethyl ether	10	1							
di-n-propyl ether	14	1							
methyl phenyl ether (anisole)	8	1							1
diphenyl ether	10	1							2
Tetrahydrofuran (1-Oxacyclopentane)	8	1							
1,4- dioxane (1,4-Dioxacyclohexane)	8	2							
acetone	6		1						
2-butanone	8		1						
2-pentanone	10		1						
2-hexanone	12		1						
2-octanone	16		1						

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	Low polarity groups	Polar groups		Hydrogen bonded groups					Aromatic rings
methyl phenyl ketone (Acetophenone)	8		1						1
diphenyl ketone (Benzophenone)	10		1						2
methanol	3			1					
Representative groups	C-H	C-O, C_3-N, C-F	C=O	OH	NH_2	COOH	C-O, C=O, C-N	NH	aromatic rings
Substance	N_{lp}	N_p	N_p	N_{hb}	N_{hb}	N_{hb}	N_{hb}	N_{hb}	N_{ar}
ethanol	5			1					
1-propanol	7			1					
1-butanol	9			1					
1-pentanol	11			1					
1-hexanol	13			1					
1-octanol	17			1					
1-dodecanol	25			1					
2-propanol	7			1					
2-butanol	9			1					
isobutanol	9			1					
phenol	5			1					1
1-Naphthalenol	7			1					2
1,2 ethanediol	4			2					
1,3 propanediol	6			2					
1,5 pentanediol	10			2					
1,4-benzenediol (hydroquinone)	4			2					1
1,2,3-propanetriol (glycerin)	5			3					
methanoic acid	1					1			
ethanoic acid	3					1			
propanoic acid	5					1			
butanoic acid	7					1			
benzoic acid	5					1			1

Table S8. Parameters used for the calculation of $\Delta H_{max}$of the 38 substances presented in Table 3.

	Low polarity groups	Polar groups		Hydrogen bonded groups					Aromatic rings
Number of sites for hydrogen bonded groups (s_{hb})	1	1	1	3	4	5	2	3	1
Representative groups	C-H	C-O, C_3-N, C-F	C=O	OH	NH_2	COOH	C-O, C=O, C-N	NH	aromatic rings
Substance	N_{lp}	N_p	N_p	N_{hb}	N_{hb}	N_{hb}	N_{hb}	N_{hb}	N_{ar}
gallic acid	2			3		1			1
quercetin	5			5			2		2
sylibin	17			5			5		3
rutin	17			1			6		2
glycine	2				1	1			
arginine	7				2	1		2	
lysine	9				2	1			
hexoses (glucose, fructose, galactose etc.)	7			5			1		
pentoses (arabinose, xylose etc)	6			4			1		
disaccharides (sucrose, lactose etc.)	14			8			3		
tartaric acid	2			2		2			
citric acid	4			1		3			
caffeic acid	5			2		1			1
ferulic acid	8			1		1	1		1
ascorbic acid (vitamin C)	4			4			2		
nicotinic acid (vitamin B3)	4	1				1			
pyridoxine (vitamin B6)	8	1		3					
α-Tocopherol (vitamin E)	49			1			1		1
amoxicillin	14	2		1	1	1	2	1	1
benzylpenicillin	16	2				1	2	1	1
levofloxacin	19	4				1	2		1
aspirin	7					1	2		1

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	Low polarity groups	Polar groups		Hydrogen bonded groups					Aromatic rings
ibuprofen	17					1			1
Representative groups	C-H	C-O, C_3-N, C-F	C=O	OH	NH_2	COOH	C-O, C=O, C-N	NH	aromatic rings
Substance	N_{lp}	N_p	N_p	N_{hb}	N_{hb}	N_{hb}	N_{hb}	N_{hb}	N_{ar}
fenoprofen	14					1	1		2
ketorolac	12	1				1	1		1
salicylic acid	4			1		1			1
thymol/carvacrol	13			1					1
eucalyptol	18	1							
geraniol	17			1					
p-cymene	14								1
terpinene	16								
cinnamaldehyde	8		1						1
alizarin	6			2			2		2
anilin	5				1				1
hypericin	1			6			2		6

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