Molecular Interactions

Issues to Study:

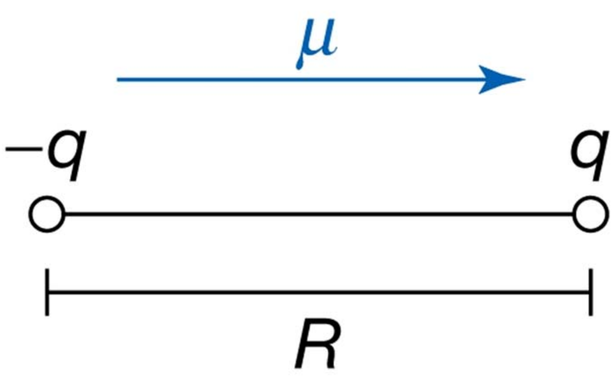
Electrical Properties

- electrical dipole moments
- polarizability
- relative permittivity and refractive index

Intermolecular Interactions

- interactions between dipoles
- repulsive interactions
- total interactions

Electrical Dipole Moments



1 Electric dipole

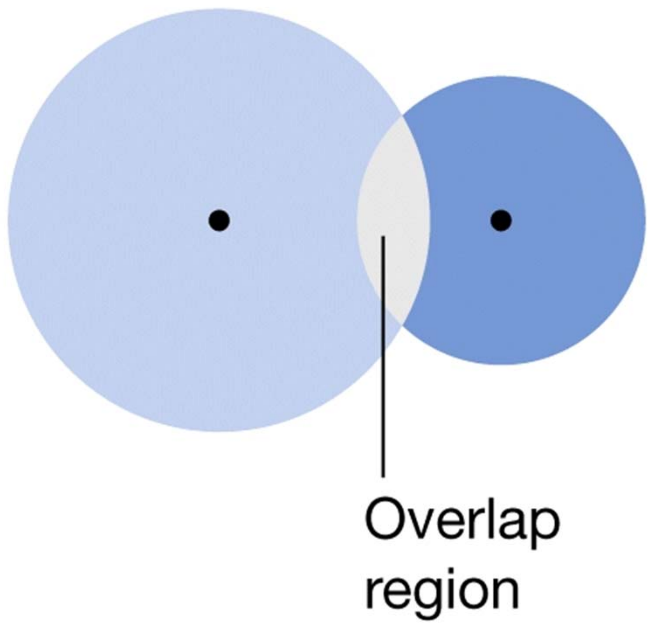


Table 21.1* Dipole moments (μ) and polarizability volumes (α')

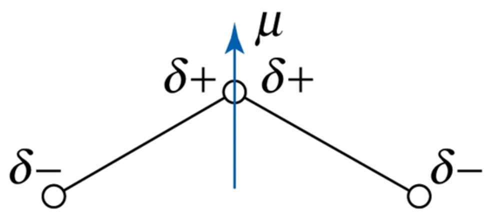
	μ/D	$\alpha'/(10^{-30}\ m^3)$
CCl_4	0	10.5
H_2	0	0.819
H_2O	1.85	1.48
HCl	1.08	2.63
HI	0.42	5.45

* More values are given in the *Data section* at the end of this volume.

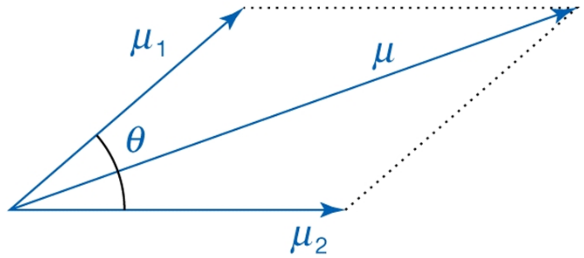
1. Dipole moment의 크기는 분자구조와 어떤 연관성을 가지는가?
2. 어떤 경우에 0이 되는가?
3. 원자의 전기음성도(electronegativity)와의 관계는?

* Professor Linus Pauling

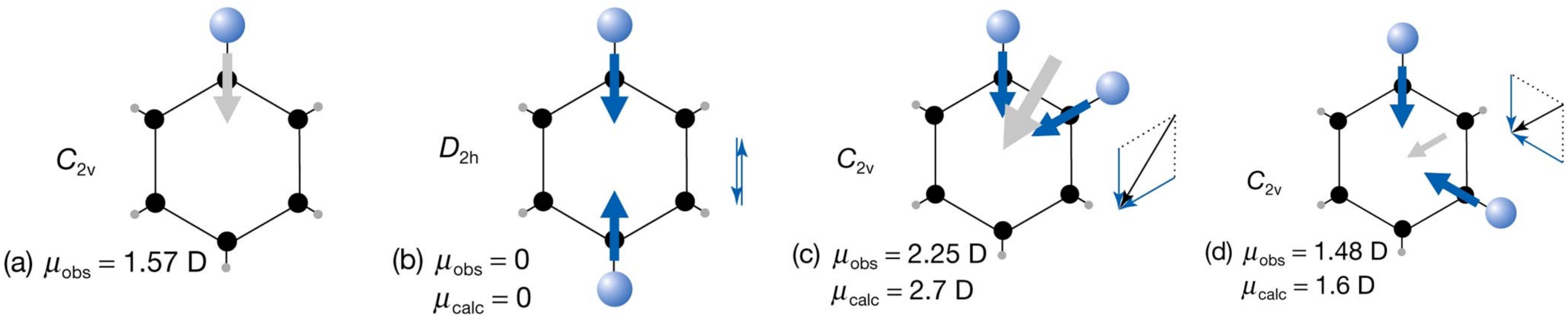
구조적인 연관성 찾기



2 Ozone, O_3

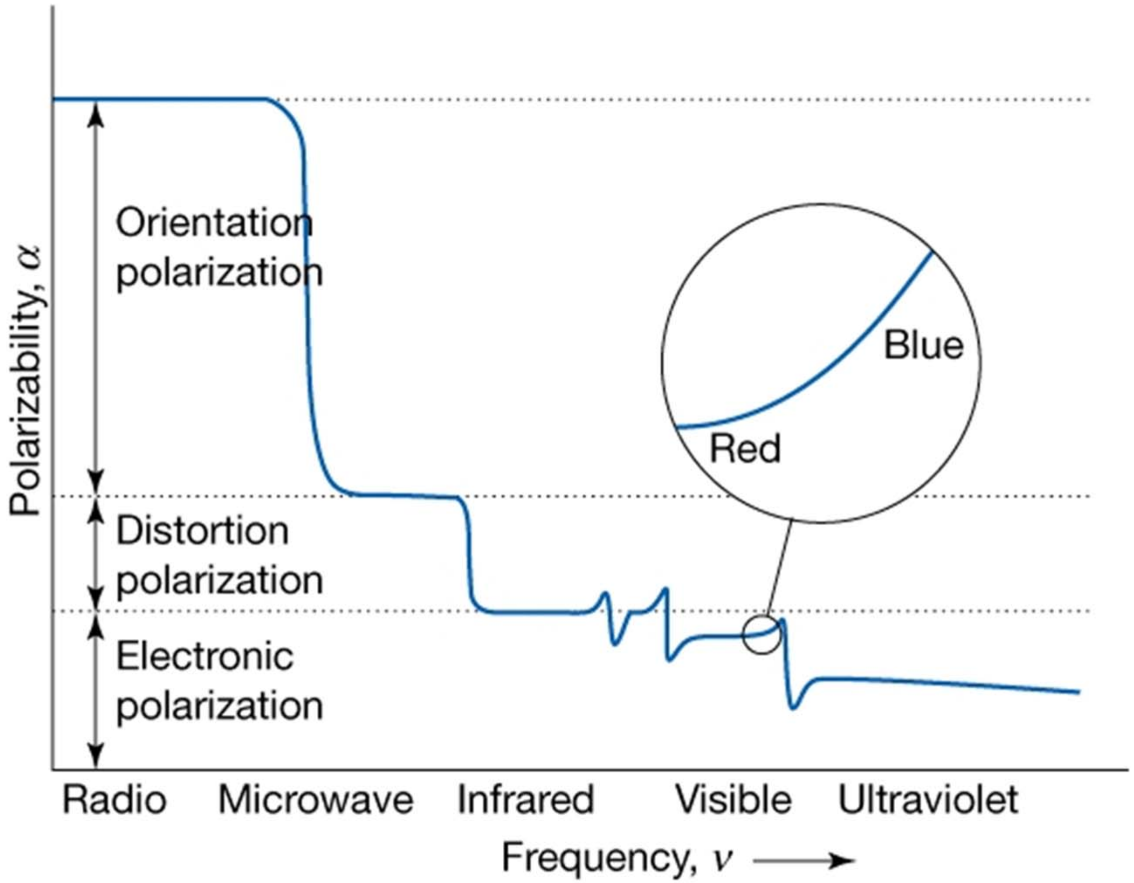


3 Addition of dipoles



Polarizability, Relative Permittivity, Refractive Index

* Clausius-Mossotti equation의 이해



Dispersion of Refractive Index

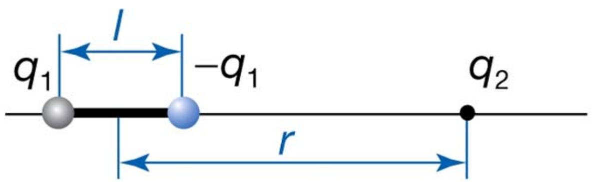
Table 21.2* Refractive indices (at different wavelengths of light) relative to air at 20°C

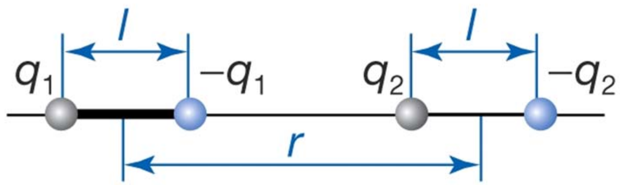
	434 nm	589 nm	656 nm
C_6H_6(l)	1.524	1.501	1.497
CS_2(l)	1.675	1.628	1.618
H_2O(l)	1.340	1.333	1.331
KI(s)	1.704	1.666	1.658

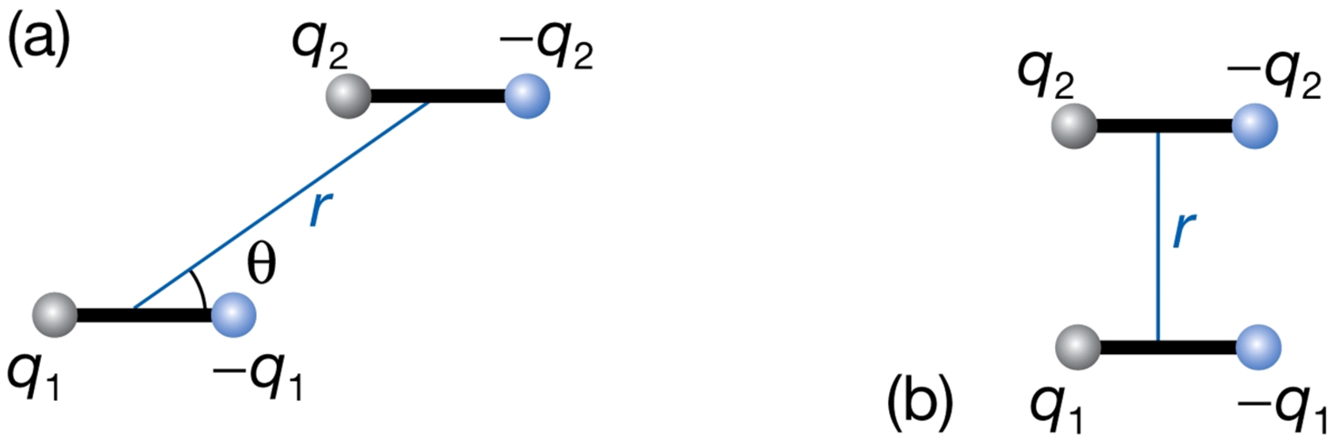
* More values are given in the *Data section*.

1. Snell's Law: incidence, reflection, refraction
2. Total internal reflection의 이해
3. Copper wire vs. Glass optic fiber vs. Plastic optic fiber

Interactions between Dipoles







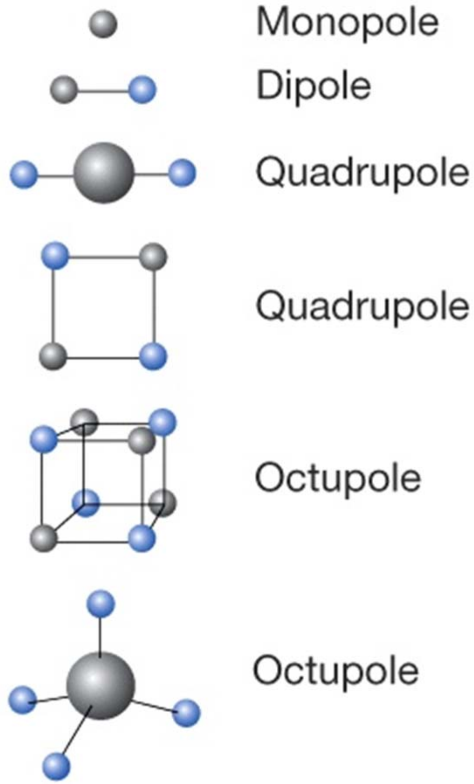
Dipole간의 거리와 방향(orientation)

Table 21.3 Multipole interaction potential energies

Interaction type	Distance dependence of potential energy	Typical energy/ (kJ mol^{-1})	Comment
Ion–ion	$1/r$	250	Only between ions*
Ion–dipole	$1/r^2$	15	
Dipole–dipole	$1/r^3$	2	Between stationary polar molecules
	$1/r^6$	0.6	Between rotating polar molecules
London (dispersion)	$1/r^6$	2	Between all types of molecules

The energy of a hydrogen bond A—H···B is typically 20 kJ mol^{-1} and occurs on contact for A, B = N, 0, or F.

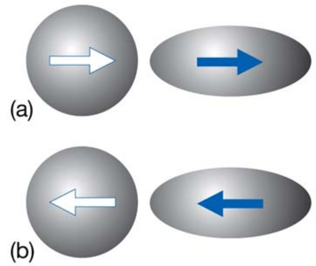
* Electrolyte solutions are treated in Chapter 10, ionic solids in Chapter 23.



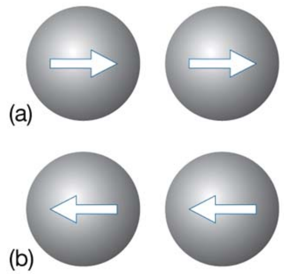
Pole의 개수와 거리와의 관계

Dipole-Dipole interaction
(Keesom interaction)

Dipole-Induced dipole interaction
(Debye interaction)



Induced dipole-Induced dipole interaction)
(London interaction, Dispersion)



Total Van der Waals attractive interaction
= Keesom + Debye + London

* Additional hydrogen-bonding can be considered.

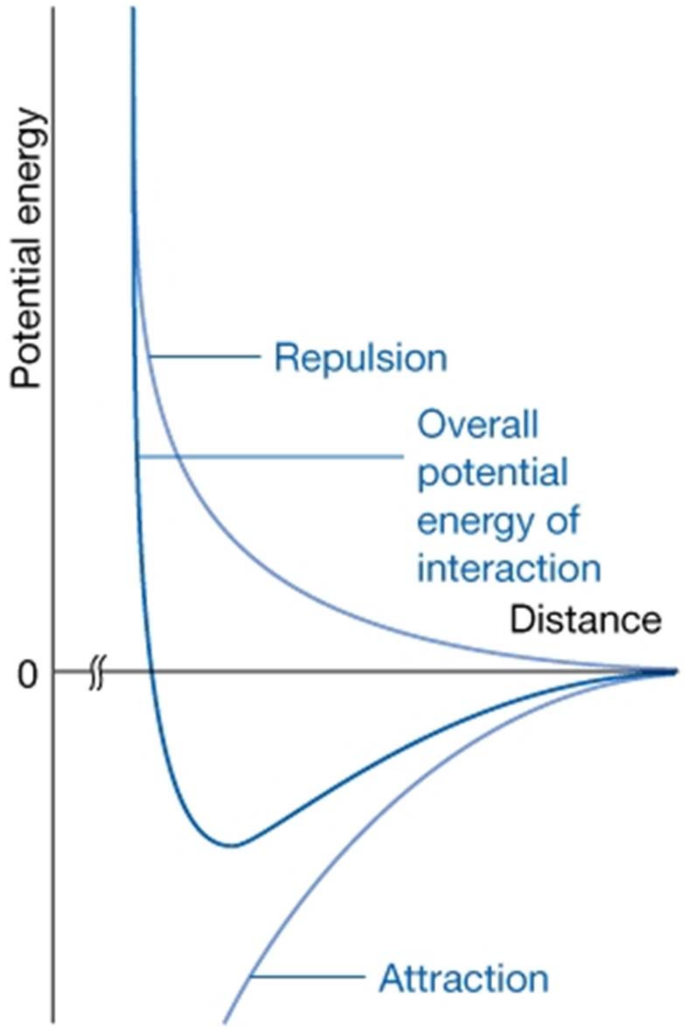
Table 11.2 Percentage of the Debye, Keesom, and London Contributions to the Van der Waals Attraction Between Various Molecules.[a]

Compound	μ (debye)	$\frac{\alpha}{4\pi\varepsilon_0} \times 10^{30}$ (m^3)	$\beta \times 10^{77}$ ($J\ m^6$)	Percentage contribution of: Keesom (permanent–permanent)	Debye (permanent–induced)	London (induced–induced)
CCl_4	0	10.7	4.41	0	0	100
Ethanol	1.73	5.49	3.40	42.6	9.7	47.6
Thiophene	0.51	9.76	3.90	0.3	1.3	98.5
t-Butanol	1.67	9.46	5.46	23.1	9.7	67.2
Ethyl ether	1.30	9.57	4.51	10.2	7.1	82.7
Benzene	0	10.5	4.29	0	0	100
Chlorobenzene	1.58	13	7.57	13.3	8.6	78.1
Fluorobenzene	1.35	10.3	5.09	10.6	7.5	81.9
Phenol	1.55	11.6	6.48	14.5	8.6	76.9
Aniline	1.56	12.4	7.06	13.6	8.5	77.9
Toluene	0.43	11.8	5.16	0.1	0.9	99.0
Anisole	1.25	13.7	7.22	5.5	6.0	88.5
Diphenylamine	1.08	22.6	14.25	1.5	3.7	94.7
Water	1.82	1.44	2.10	84.8	4.5	10.5

[a]Dipole moments and polarizabilities from A. L. McClellan, *Tables of Experimental Dipole Moments*, Freeman, San Francisco, 1963.

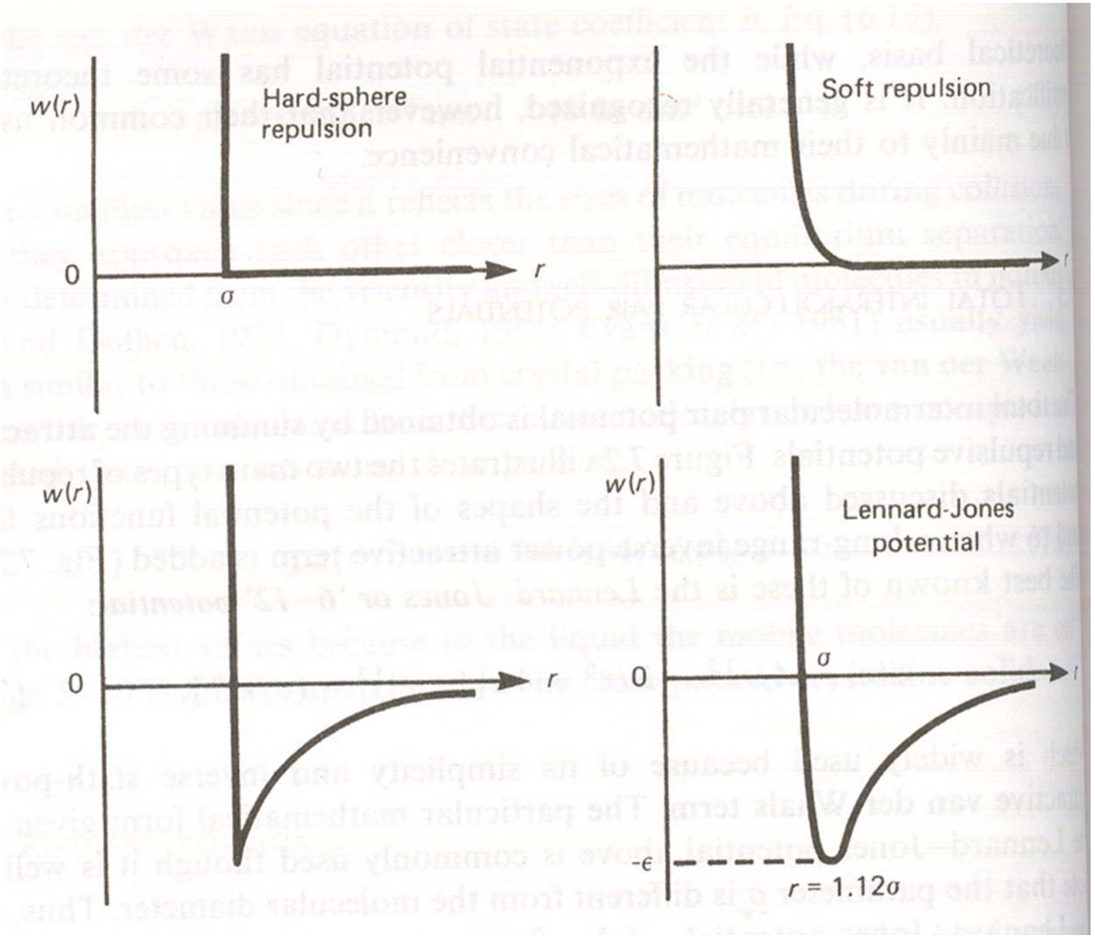
1. Dipole moment와 polarizability의 크기에 따른 VDW의 변화
2. 각 분자의 특성에 따른 Keesom, Debye, London의 구성 비율
3. London interaction의 중요성
4. 물의 특이성

Overall Potential Energy



*Potential vs distance curve로 부터
Force vs distance curve 도출

Various Models for Overall Potential



* 각 모델의 의미를 생각해 보고 수학적으로 표현하기

Lennard-Jones 12,6 Potential

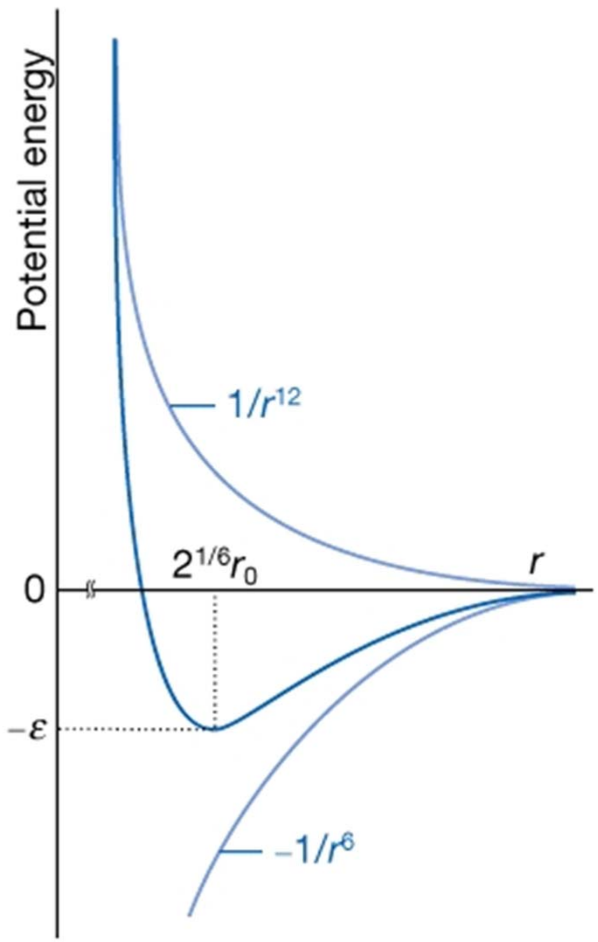


Table 21.4* Lennard-Jones (12, 6) parameters

	(ε/k)/K	r_0/pm
Ar	111.84	362.3
CCl_4	376.86	624.1
N_2	91.85	391.9
Xe	213.96	426.0

* More values are given in the *Data section*.
† ε is expressed as an effective temperature on division by Boltzmann's constant *k*.