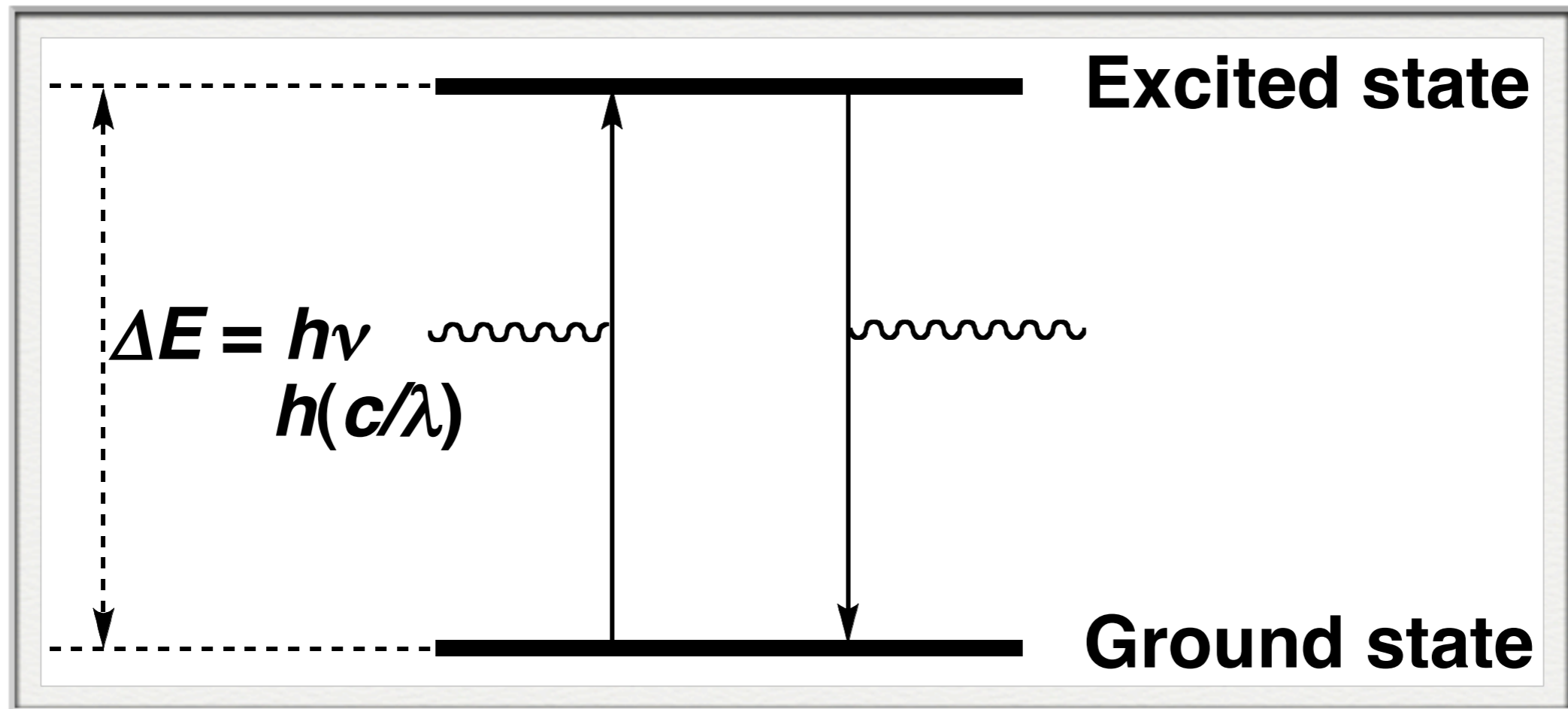


Infrared Spectroscopy (赤外分光法)

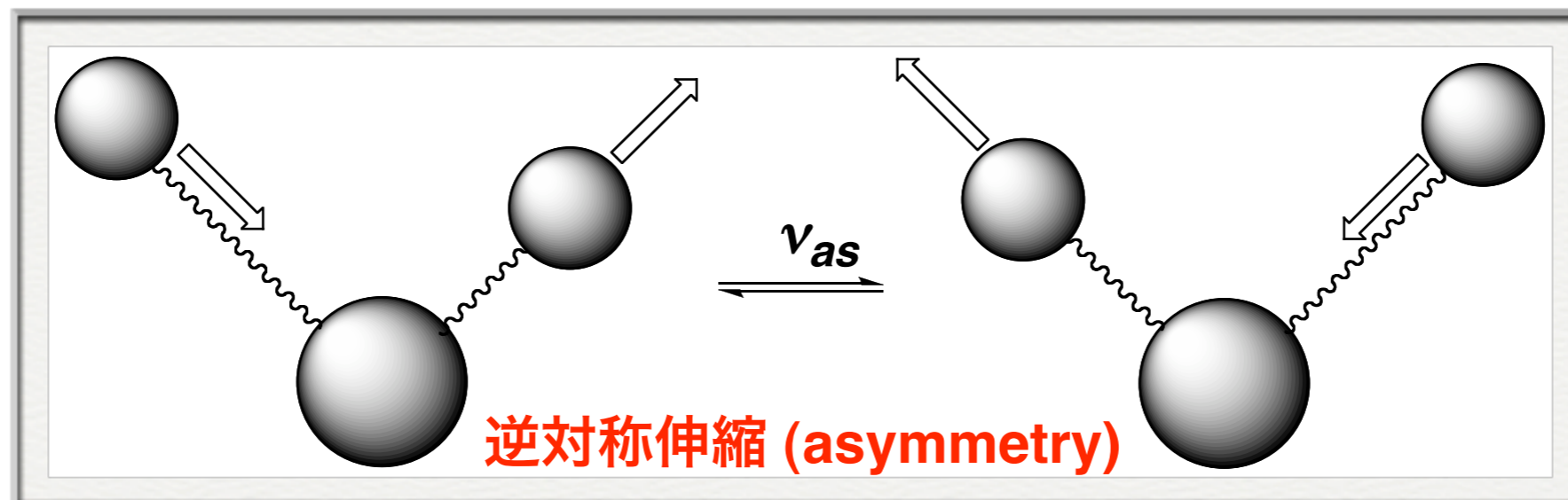
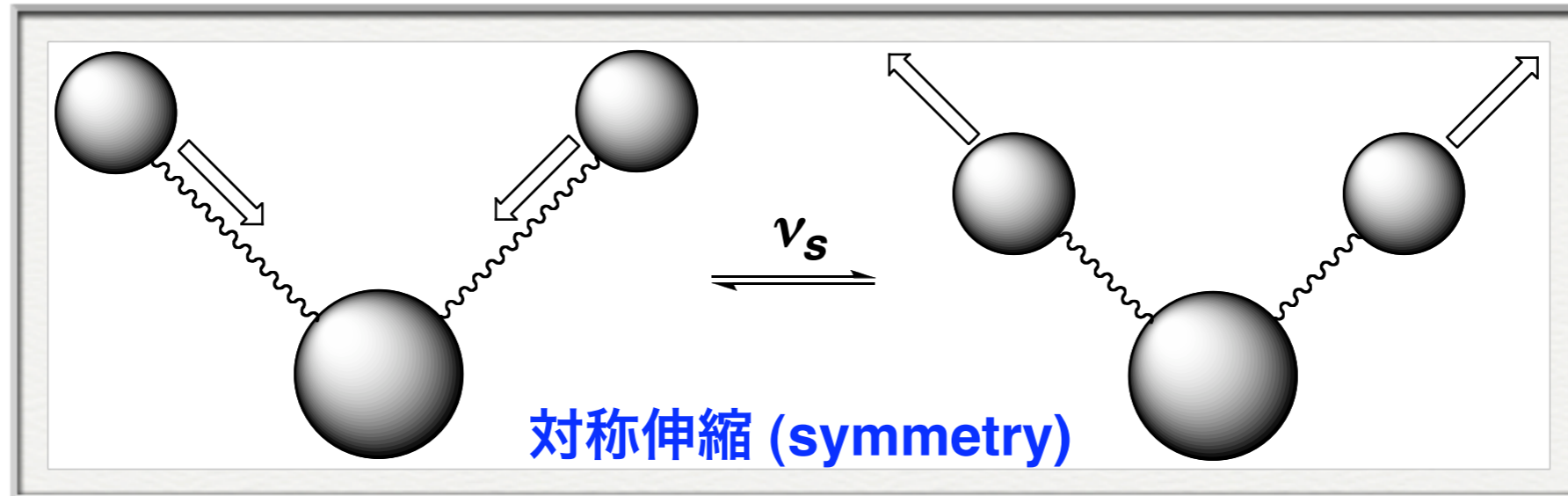
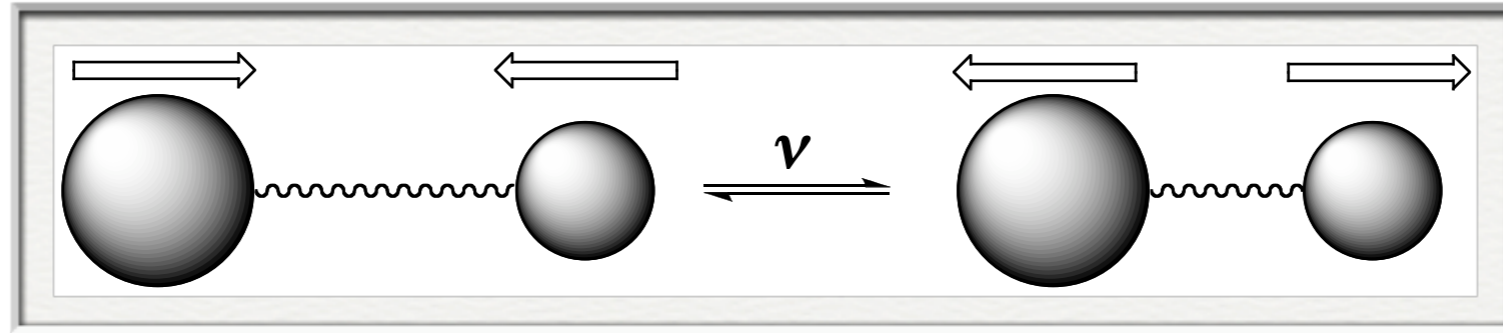
振動遷移 (vibrational transition)



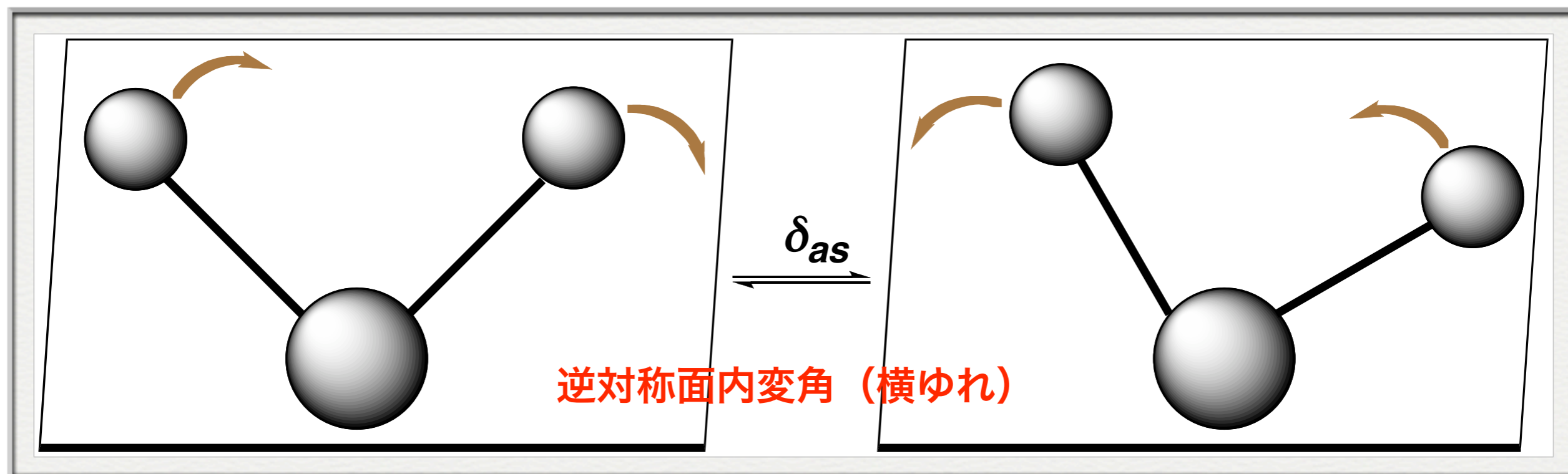
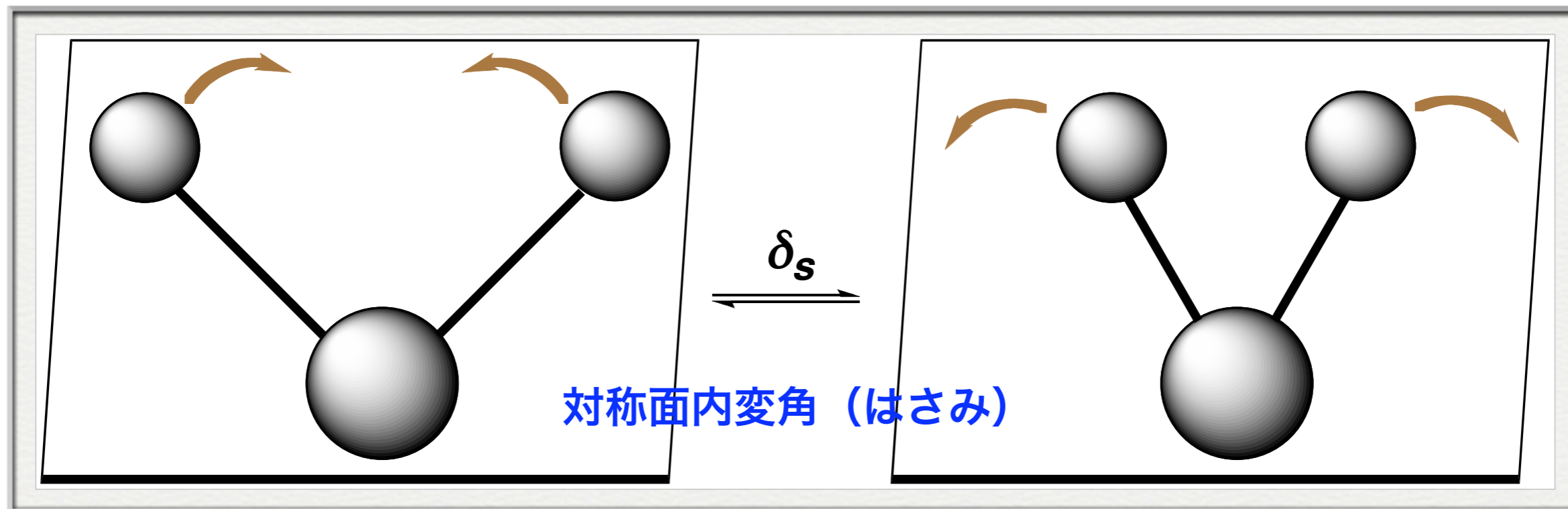
$$\lambda = 2.5 \sim 25 \mu\text{m} \text{ 赤外線}$$

$$\frac{1}{\lambda} = \tilde{\nu} = 4000 \sim 400 \text{ cm}^{-1} \dots \text{波数 または カイザー}$$

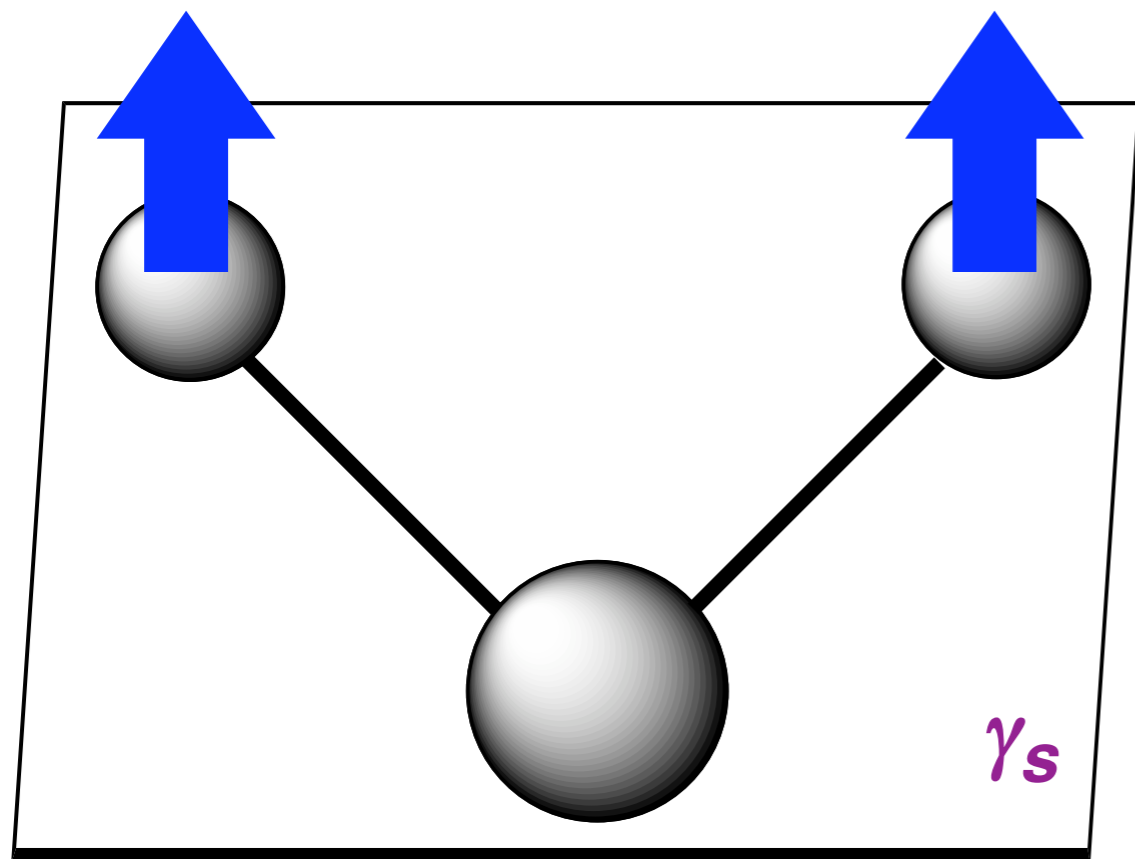
伸縮振動 (stretching)



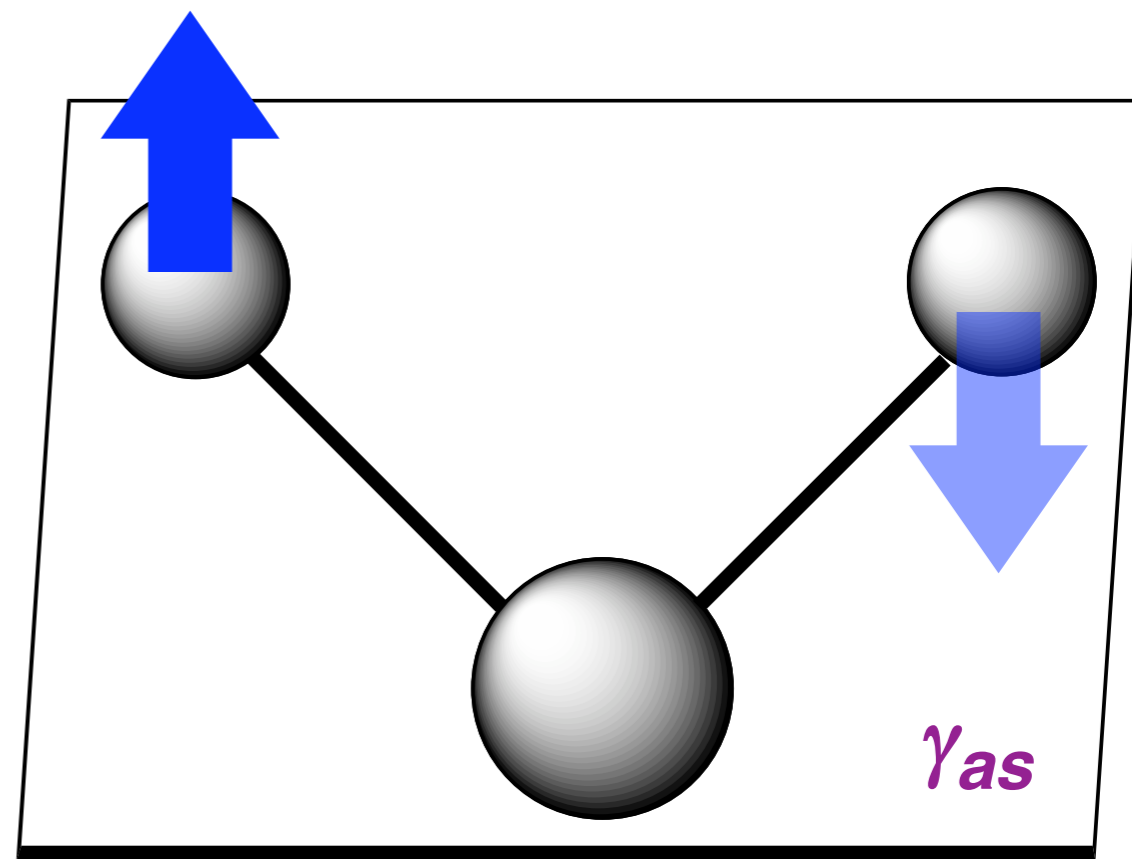
面内変角振動 (vending)



面外変角振動 (vending)



対称面外変角 (縦揺れ)



逆対称面外変角 (ひねり)

吸収波数（フックの法則）

結合のポテンシャルエネルギー: $V(r) = \frac{1}{2} kx^2$

k : 力の定数 \approx 結合の強さ

結合の振動数: $\tilde{\nu} = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}$, $\mu = \frac{m_1 m_2}{m_1 + m_2}$ (換算質量)

ポイント (μ と k の兼ね合い)

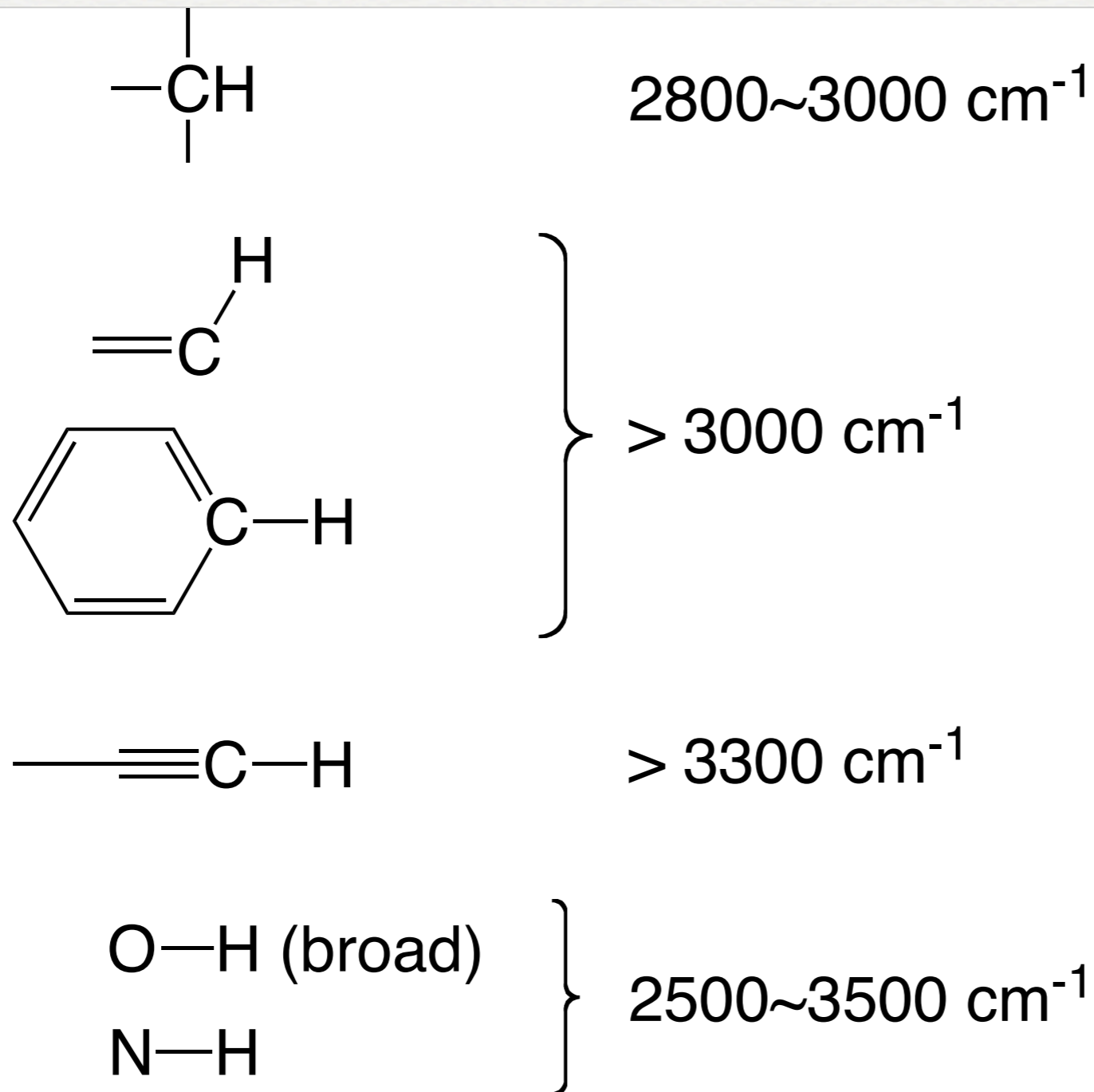
1. $\tilde{\nu}(\text{stretching}) > \tilde{\nu}(\text{bending})$

2. $\tilde{\nu}(\text{C} \equiv \text{C}) > \tilde{\nu}(\text{C} = \text{C}) > \tilde{\nu}(\text{C} - \text{C})$

3. $\tilde{\nu}(\text{C-H}) > \tilde{\nu}(\text{C-C})$, $\tilde{\nu}(\text{O-H}) > \tilde{\nu}(\text{C-O})$, $\tilde{\nu}(\text{O-H}) > \tilde{\nu}(\text{C-H})$

4000 cm^{-1} ~ 2500 cm^{-1}

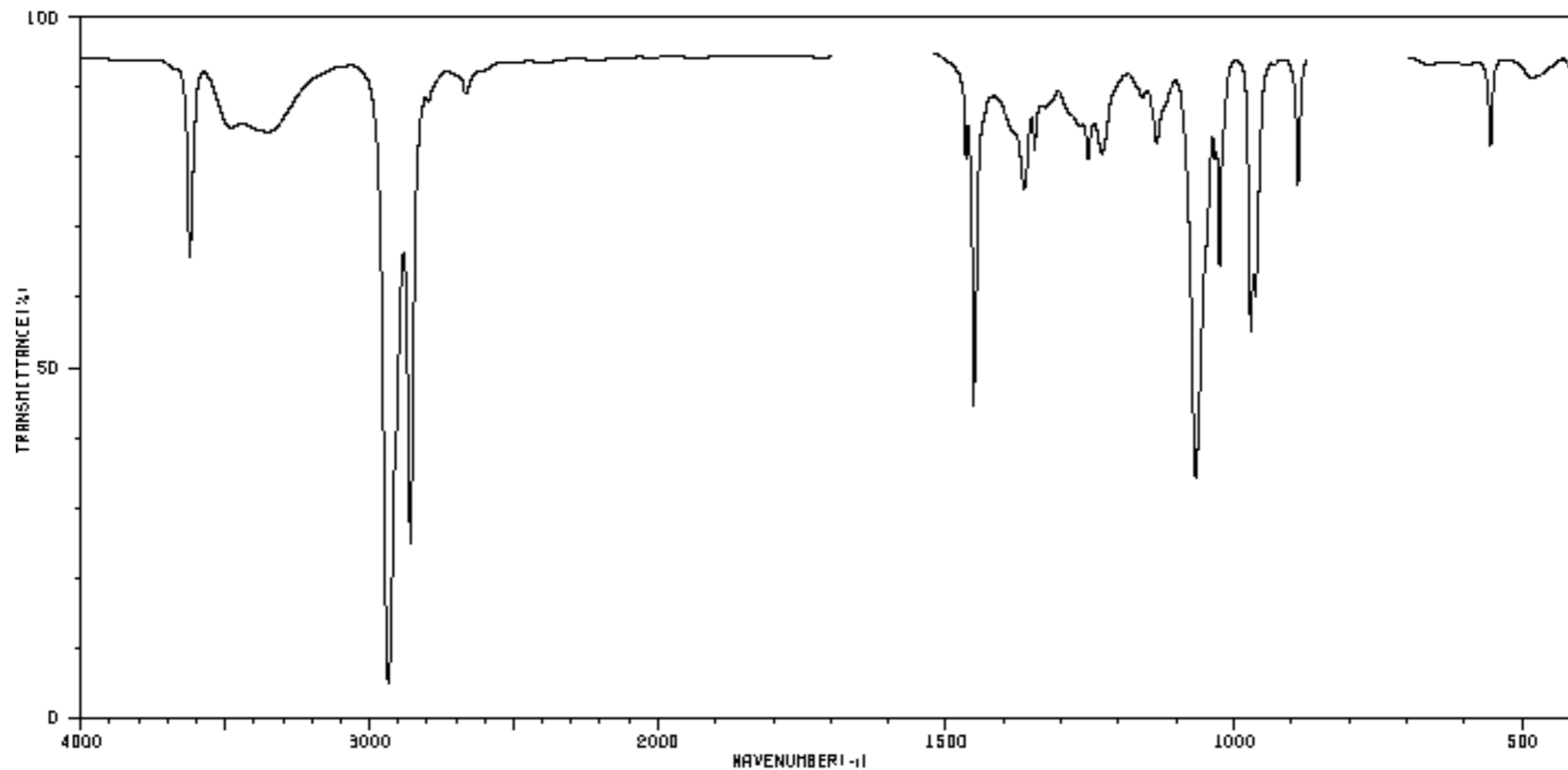
(O-H, N-H, C-H伸縮)



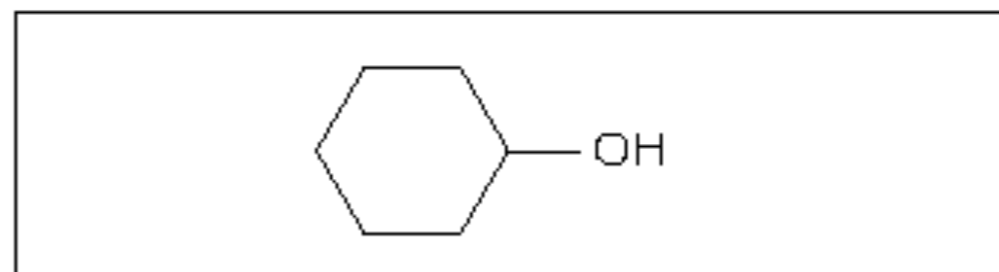
結合の強さを反映

アルコールのO-H伸縮振動 (solution)

HIT-NO=968	SCORE= ()	SDBS-NO=581	IR-NIDA-08688 : CCL4 SOLUTION
CYCLOHEXANOL			
C ₆ H ₁₂ O			

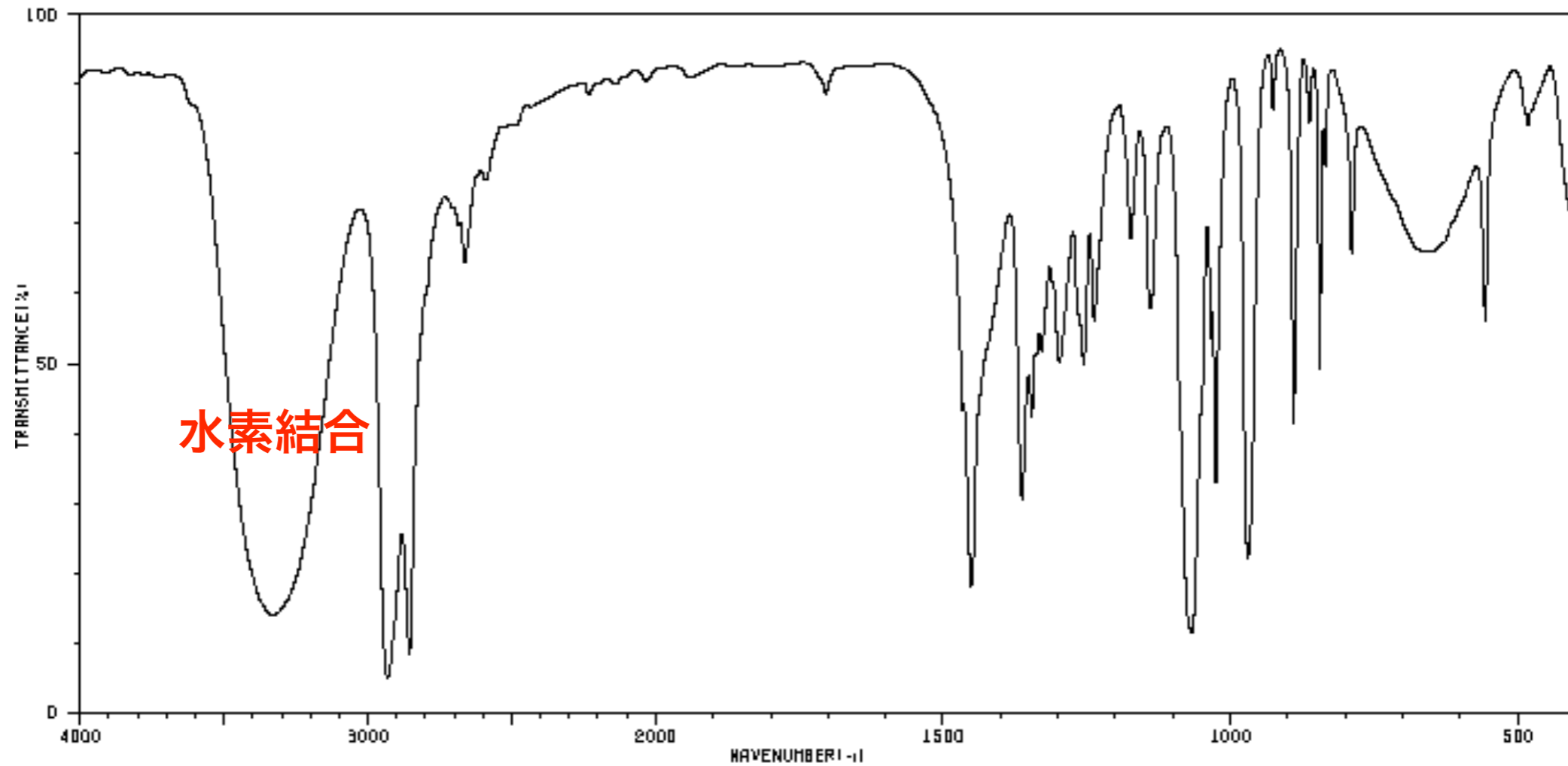


3623	62	1347	79	971	63
2934	4	1254	77	963	58
2858	23	1230	77	889	72
2666	86	1160	84	665	79
1466	77	1135	79		
1453	43	1067	39		
1365	72	1026	62		



アルコールのO-H伸縮振動 (neat)

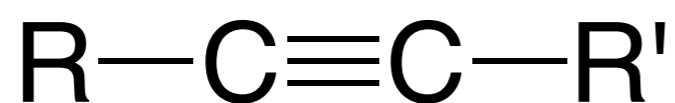
HIT-NO=1077	SCORE= ()	SDBS-NO=581	IR-NIDA-09018 : LIQUID FILM
CYCLOHEXANOL			
C ₆ H ₁₂ O			



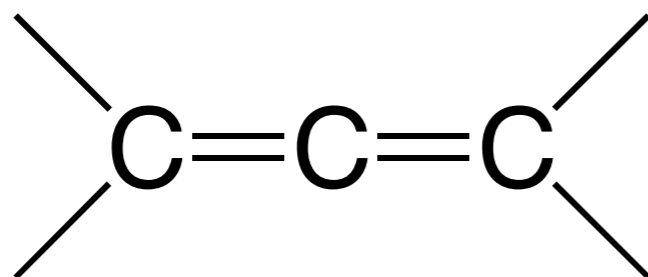
3331	13	1704	86	1256	47	970	21	657	54
2932	4	1467	42	1238	53	926	84	557	53
2855	6	1452	17	1174	86	890	39	462	61
2686	68	1363	29	1140	55	863	81		
2666	62	1346	41	1068	11	845	47		
2588	74	1329	50	1034	52	835	74		
2233	84	1298	48	1026	32	789	64		

2500 cm⁻¹ ~ 1900 cm⁻¹

(不毛な領域)



対称分子は赤外不活性

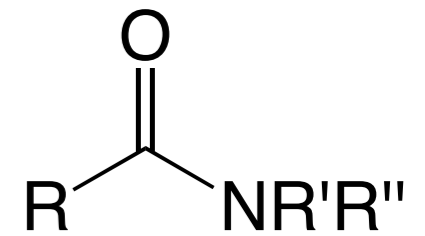
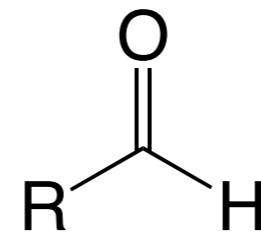
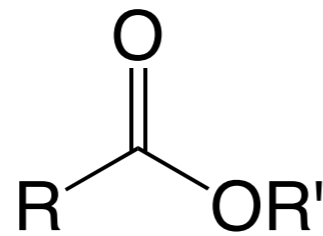
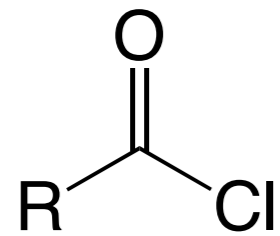
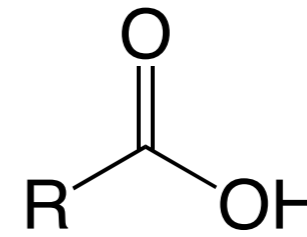
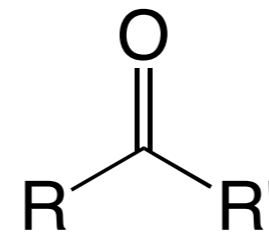
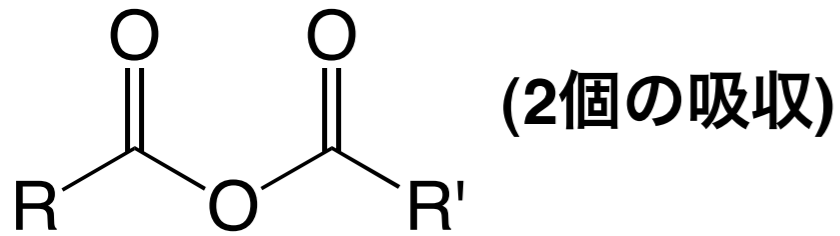


累積二重結合



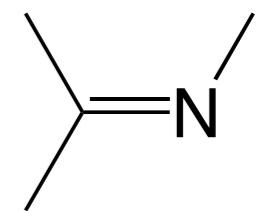
1900 cm^{-1} ~ 1500 cm^{-1}

(**C=O**, **C=C**, **C=N** 伸縮、NH変角)



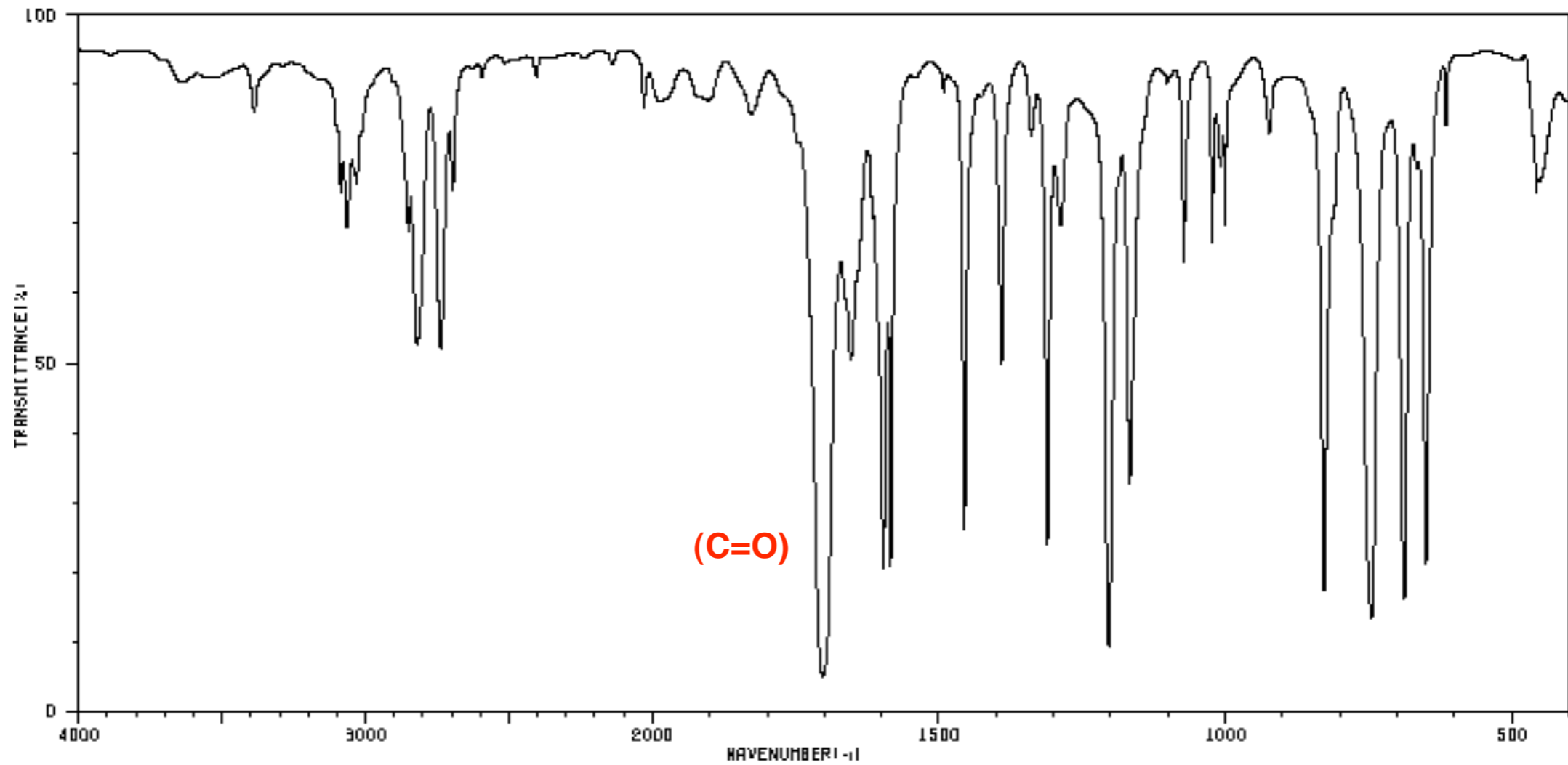
1800

1700

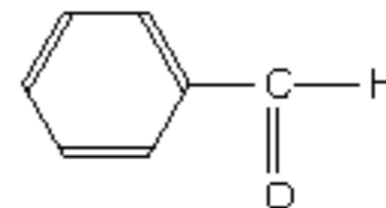


C=O伸縮振動

HIT-NO=1117	SCORE= ()	SDBS-NO=672	IR-NIDA-05223 : LIQUID FILM
BENZALDEHYDE			
C ₇ H ₆ O			



3086	72	1981	84	1697	20	1204	8	828	16
3065	66	1916	84	1584	20	1168	31	746	13
3031	72	1909	84	1456	25	1073	62	688	15
2860	66	1901	84	1391	47	1023	64	667	74
2820	50	1828	81	1339	79	1008	74	650	20
2736	50	1703	4	1311	23	1001	66	615	61
2696	72	1664	48	1288	68	924	78	457	72



$1500\text{ cm}^{-1} \sim 600\text{ cm}^{-1}$

(指紋領域: 複雑)

ν (NO): $1550 \sim 1350\text{ cm}^{-1}$ (nitro, nitroso groups)

ν (SO): $1350 \sim 1120\text{ cm}^{-1}$ (sulfones, sulfoxides)

ν (C-O): $1300 \sim 1000\text{ cm}^{-1}$ (alcohols, ethers, esters)

δ (CH): $1000 \sim 680\text{ cm}^{-1}$ (alkenes, aromatics)

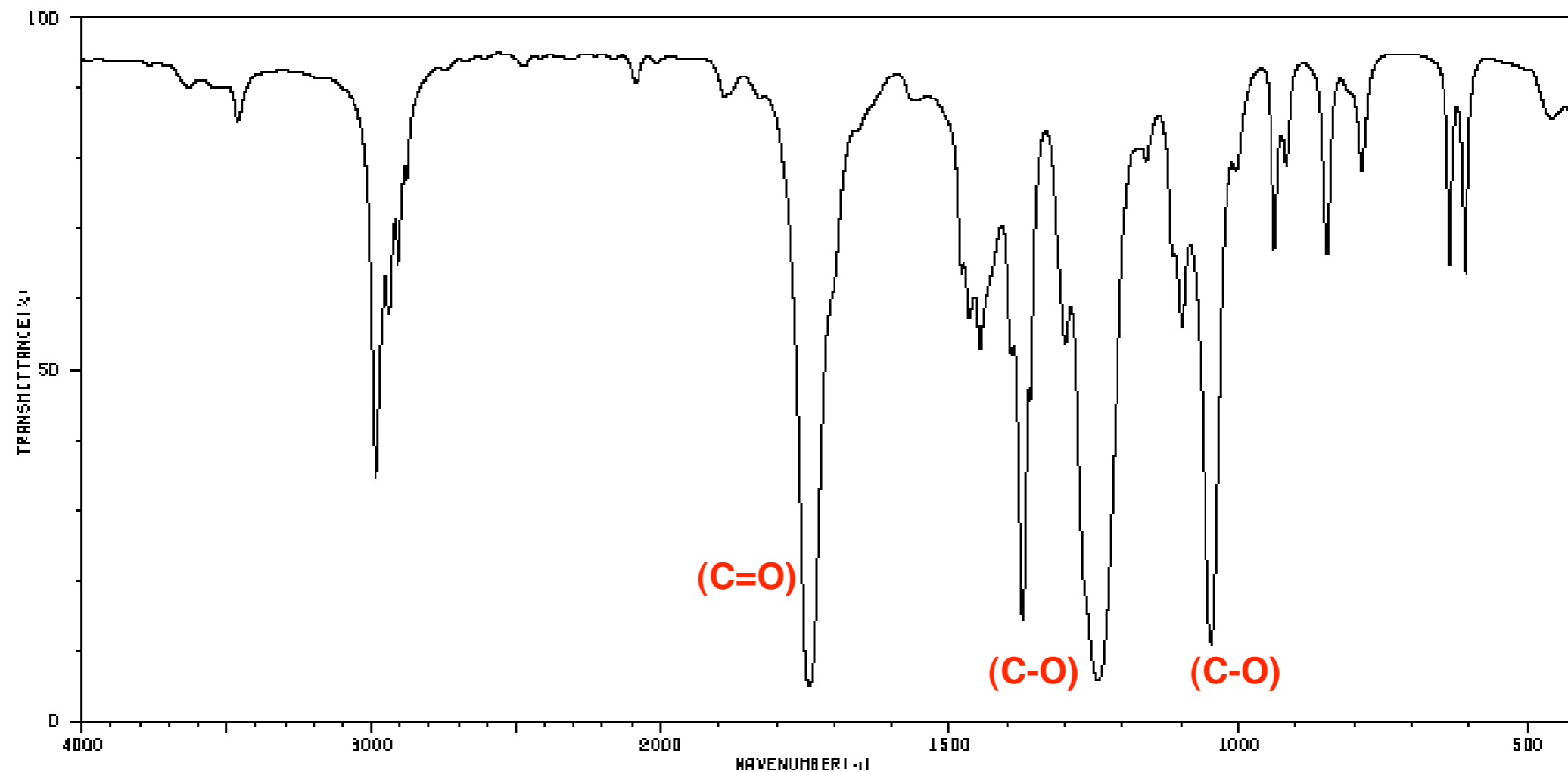
★ ケトンとエステルの区別

★ ベンゼンの置換パターン

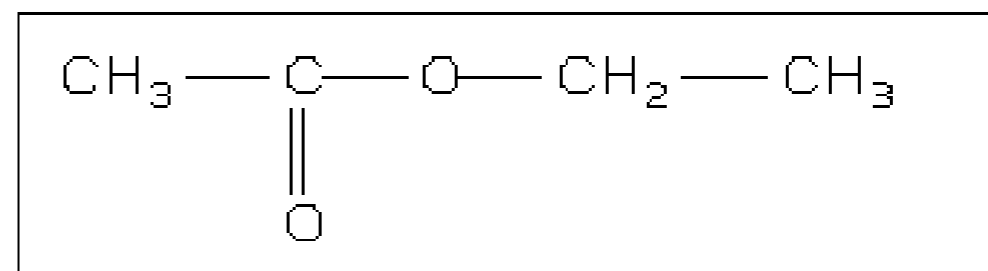
★ アルケンの置換パターン

C-O伸縮振動 (ester, 2本)

HIT-NO=1229	SCORE= ()	SDBS-NO=889	IR-NIDA-01804 : LIQUID FILM
ETHYL ACETATE			
C ₄ H ₈ O ₂			

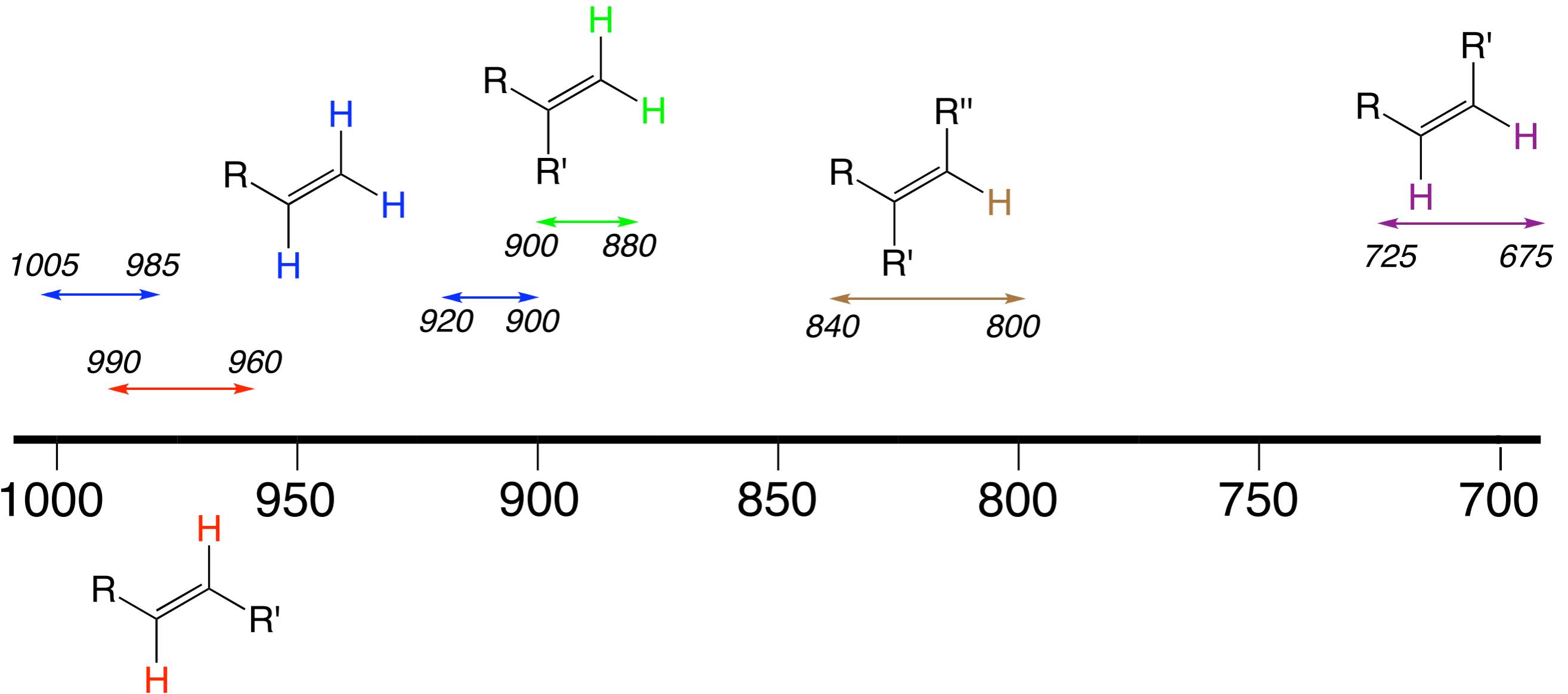


3462	81	1480	60	1243	6	847	64
2983	33	1466	55	1160	77	786	74
2940	55	1448	50	1111	84	634	62
2908	62	1393	50	1098	63	608	60
2877	74	1374	13	1048	10	457	81
1889	86	1360	49	939	84		
1743	4	1301	52	917	77		



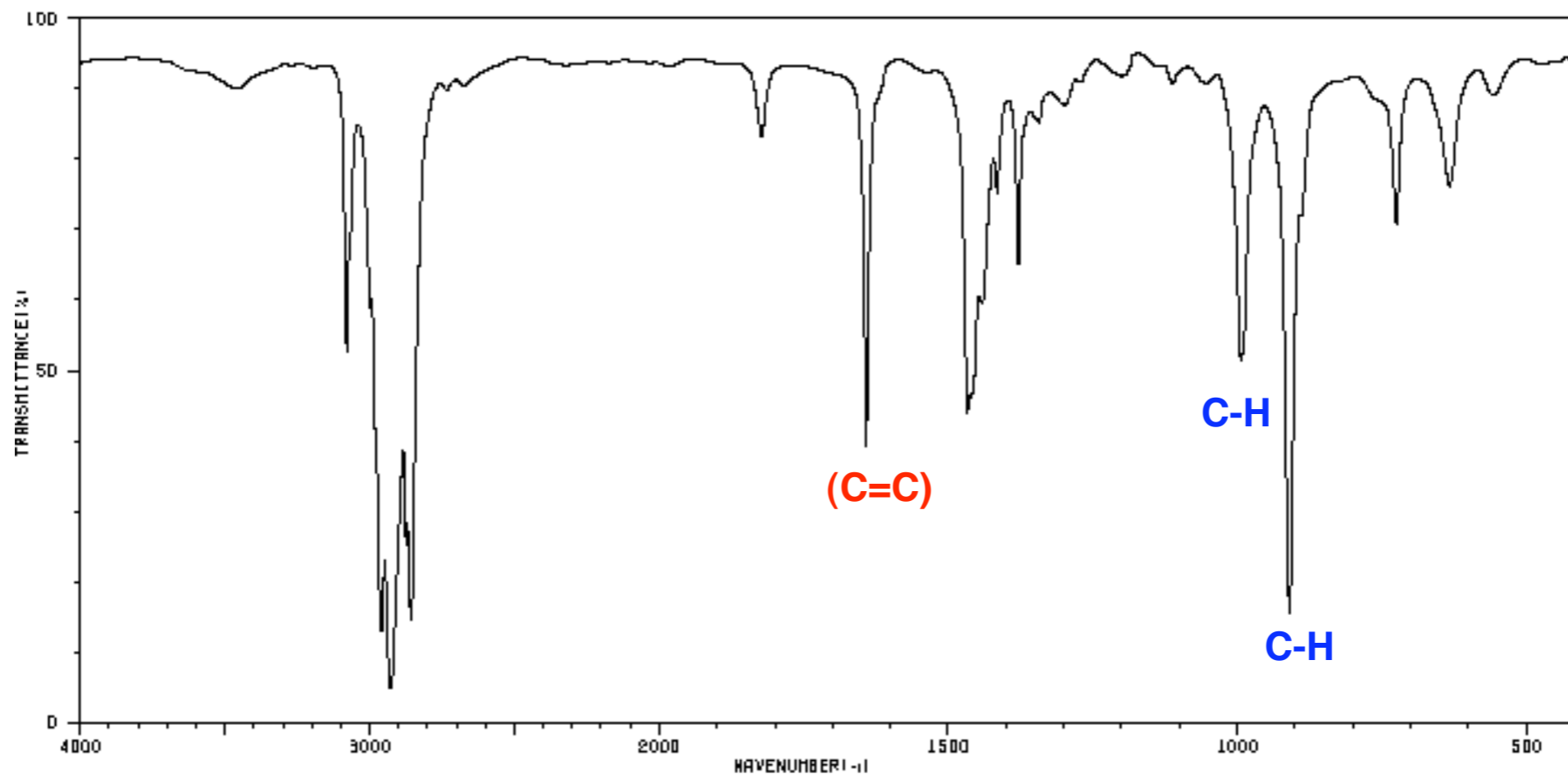
置換パターンに関する情報 (1)

(C=C)



C-H変角振動 (terminal alkenes)

HIT-NO=1179	SCORE= ()	SDBS-NO=788	IR-NIDA-04793 : LIQUID FILM
1-OCTENE			
C ₈ H ₁₆			



3079	60	1642	37	994	49
2998	57	1468	42	910	14
2959	12	1460	44	725	88
2928	4	1416	72	633	72
2874	23	1379	62	558	88
2857	13	1344	61		
1823	79	1299	84		

