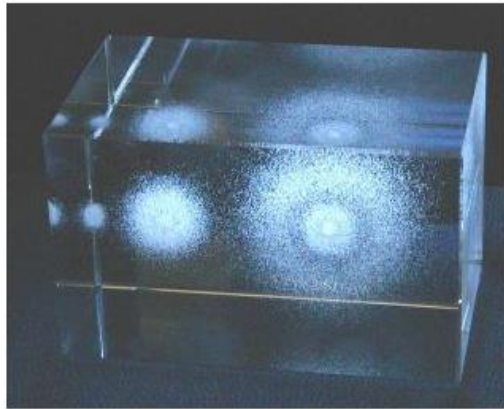
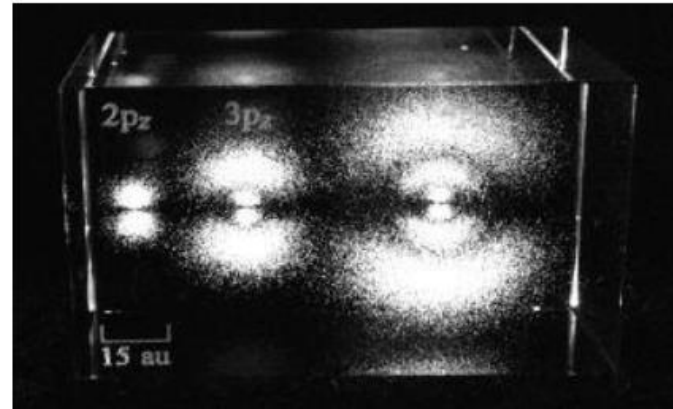


原子軌道の形とエネルギー準位

水素原子軌道のイメージ模型



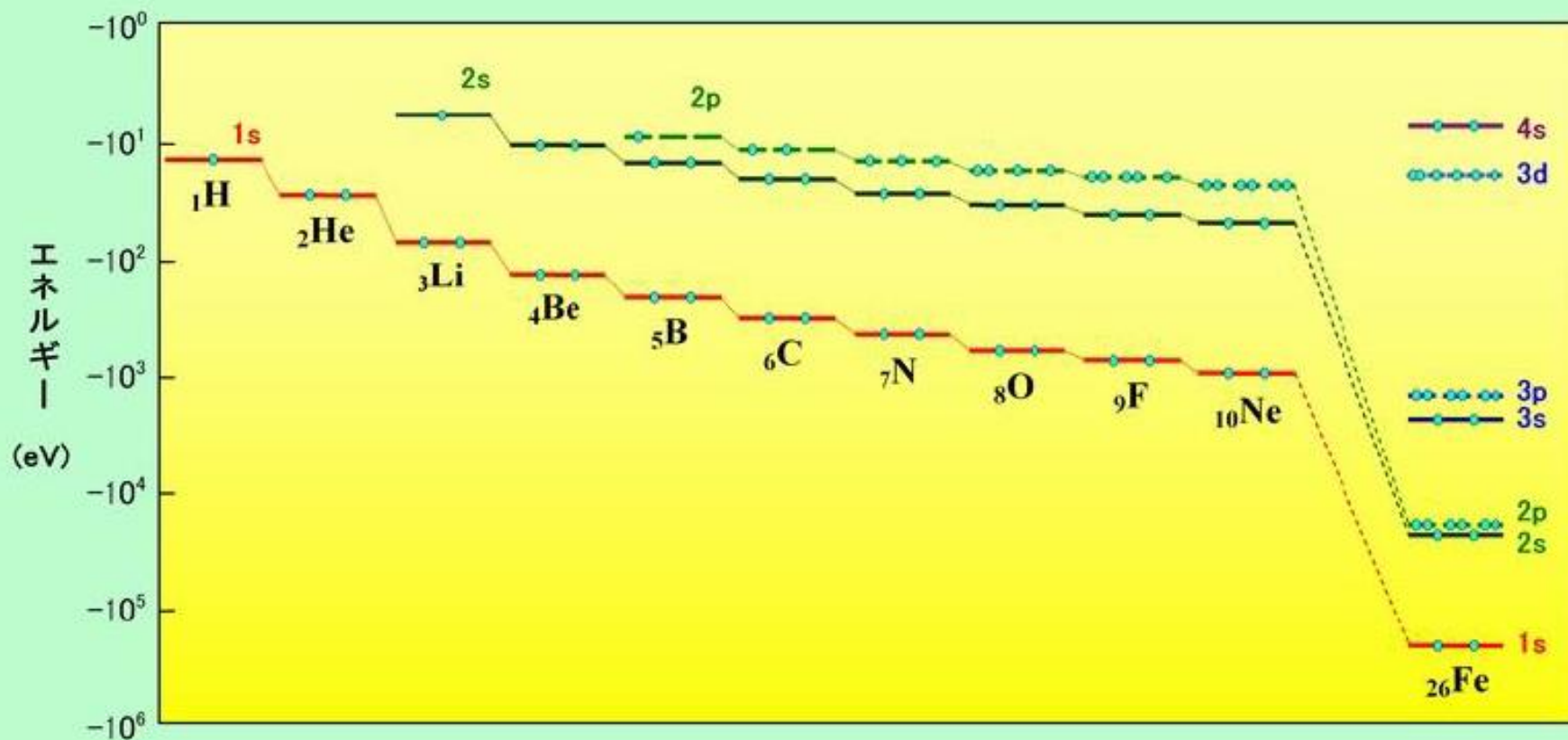
左から, 1s, 2s, 3s軌道



左から, 2p, 3p, 4p軌道

NEBULA社HP (http://winmostar.com/nebula/index_cover.html) より

原子軌道の形とエネルギー準位



原子軌道の形とエネルギー準位

イオン化エネルギー(第一イオン化ポテンシャル)

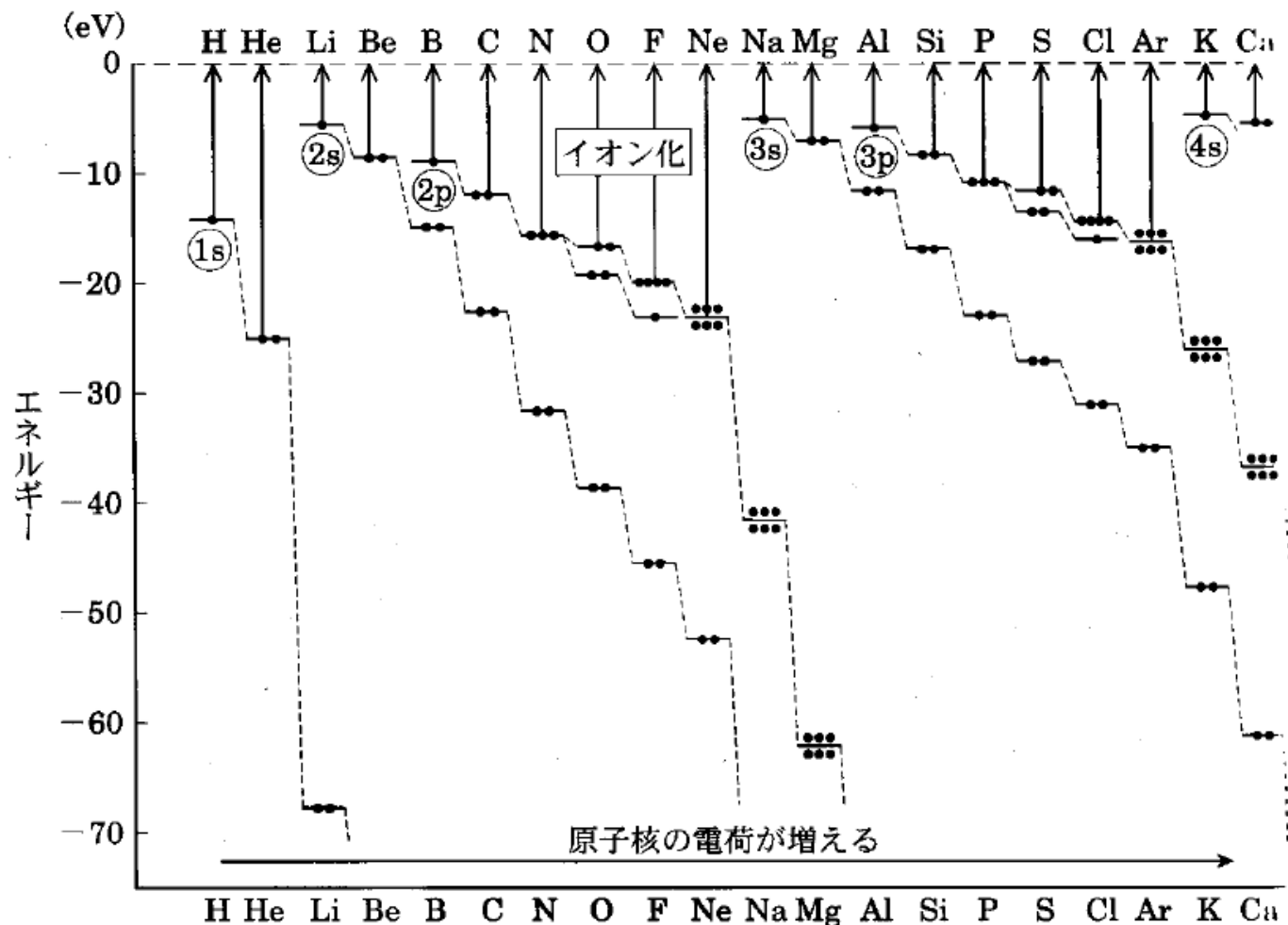
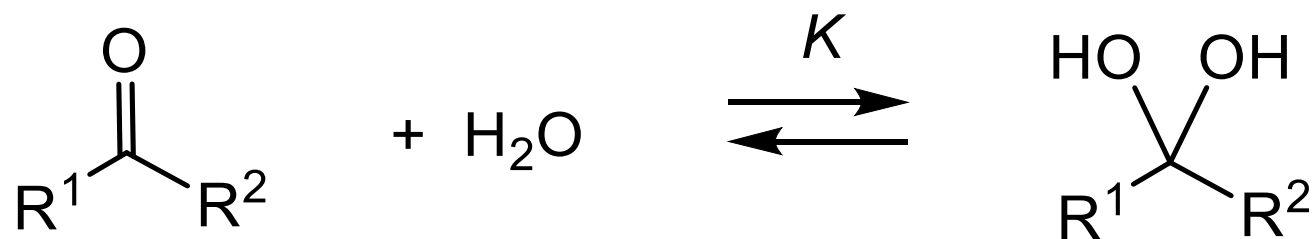
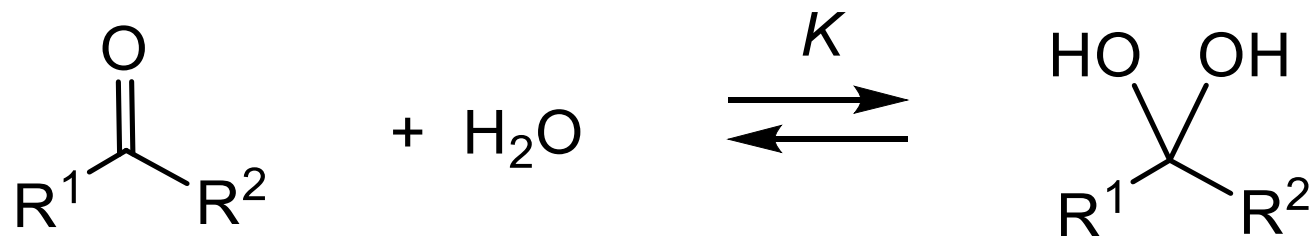


図6 水素(原子番号1)～カルシウム(20)の電子エネルギー準位(計算値)

カルボニル化合物の水和について

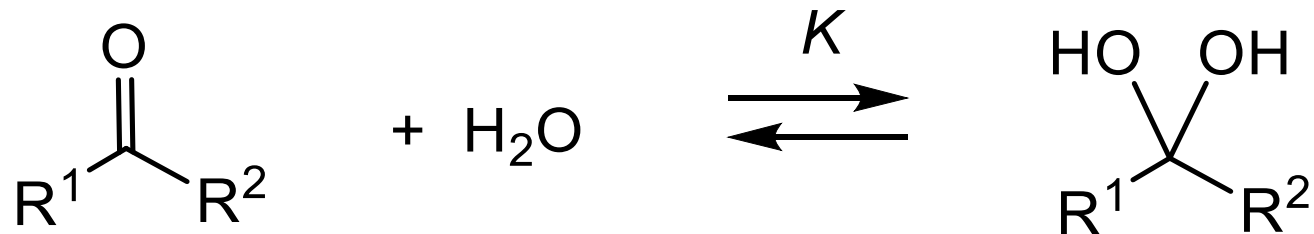


カルボニル化合物の種類の影響



R ¹	R ²	rel. <i>K</i>	LUMO level (calc.) / eV	Partial charge on carbonyl carbon (calc.)	Δ <i>H</i> _f of carbonyl compound (calc.) / kcal mol ⁻¹
CH ₃	CH ₃	0.001	0.7970	+0.2787	-52.98
CH ₃	H	1.06	0.8226	+0.2784	-44.19
H	H	2280	0.8266	+0.2971	-34.08
CCl ₃	H	2500	-0.3919	+0.2578	-51.89
CF ₃	CF ₃	1.2 × 10 ⁶	-1.5654	+0.2882	-340.02

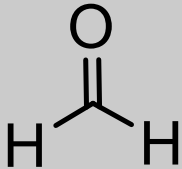
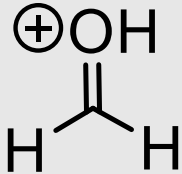
カルボニル化合物の種類の影響(2)



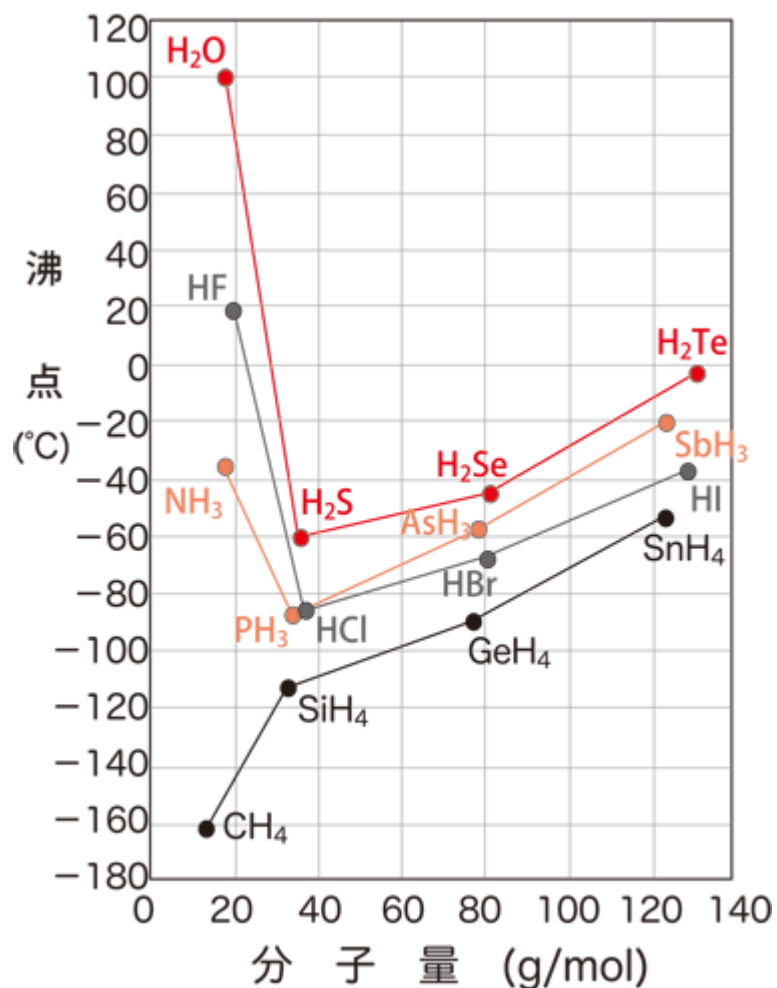
R¹	R²	rel. <i>K</i>	$\Delta H_f(\text{calc.})$ for C=O / <i>kcal mol⁻¹</i>	$\Delta H_f(\text{calc.})$ for hydrate/ <i>kcal mol⁻¹</i>	$\Delta H_r(\text{calc.})$ <i>kcal mol⁻¹</i>
CH ₃	CH ₃	0.001	-52.98	-115.57	-62.59
CH ₃	H	1.06	-44.19	-107.97	-63.78
H	H	2280	-34.08	-100.07	-65.99
CCl ₃	H	2500	-51.89	-117.72	-65.83
CF ₃	CF ₃	1.2×10^6	-340.02	-413.50	-73.48

cf. $\Delta H_f(\text{calc.})$ for H₂O = -53.42 *kcal mol⁻¹*

酸・塩基による反応加速

species	Energy level (calc.)/ eV	Partial Charge (calc.)
	0.8266 (LUMO)	+0.2971 (C)
	-7.8863 (LUMO)	+0.4718 (C)
H ₂ O	-12.3165 (HOMO)	-0.3586 (O)
OH ⁻	-1.0104 (HOMO)	-1.0553 (O)

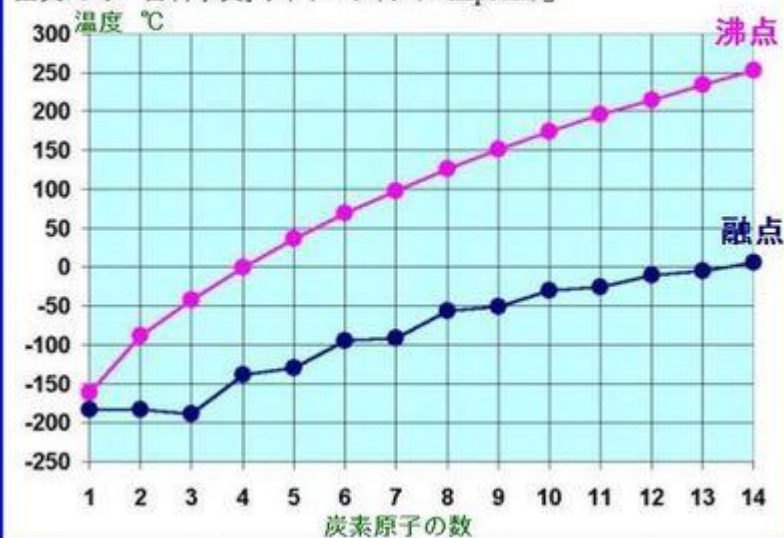
いろいろな化合物の沸点



水素化合物の沸点と分子量

直鎖のアルカンの沸点・融点

出典: フリー百科事典『ウィキペディア (Wikipedia)』





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