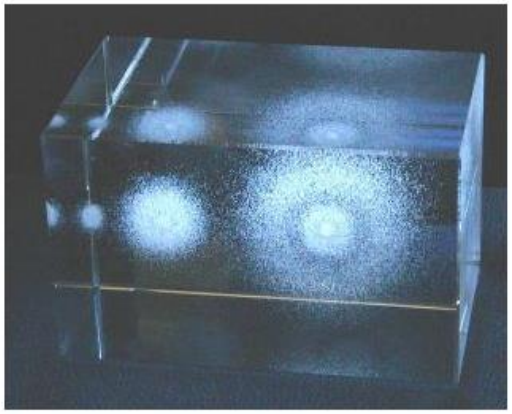
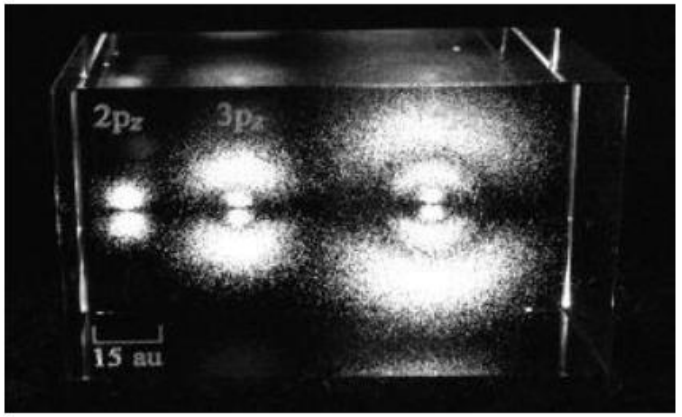
# 原子軌道の形とエネルギー準位

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

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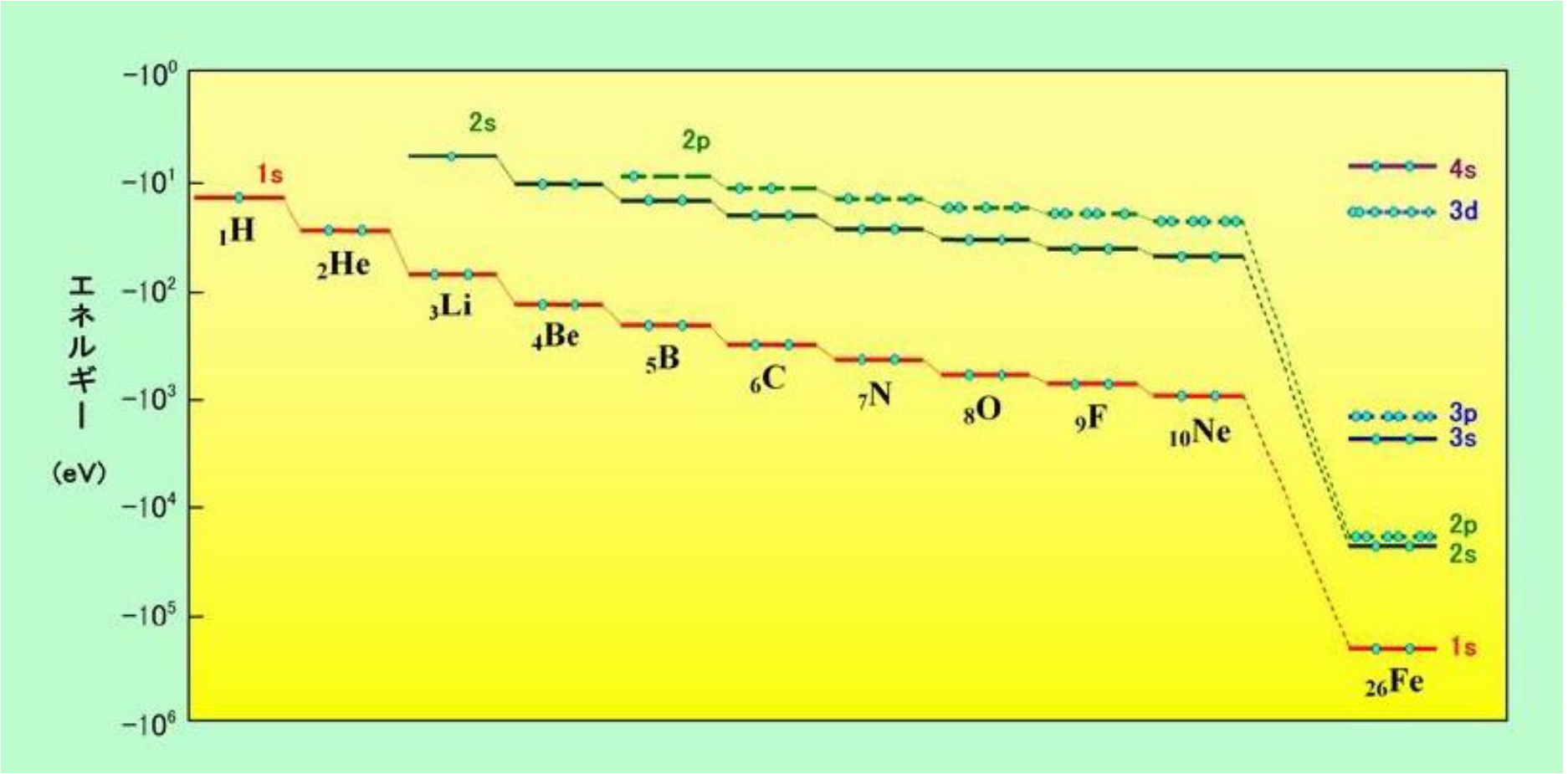

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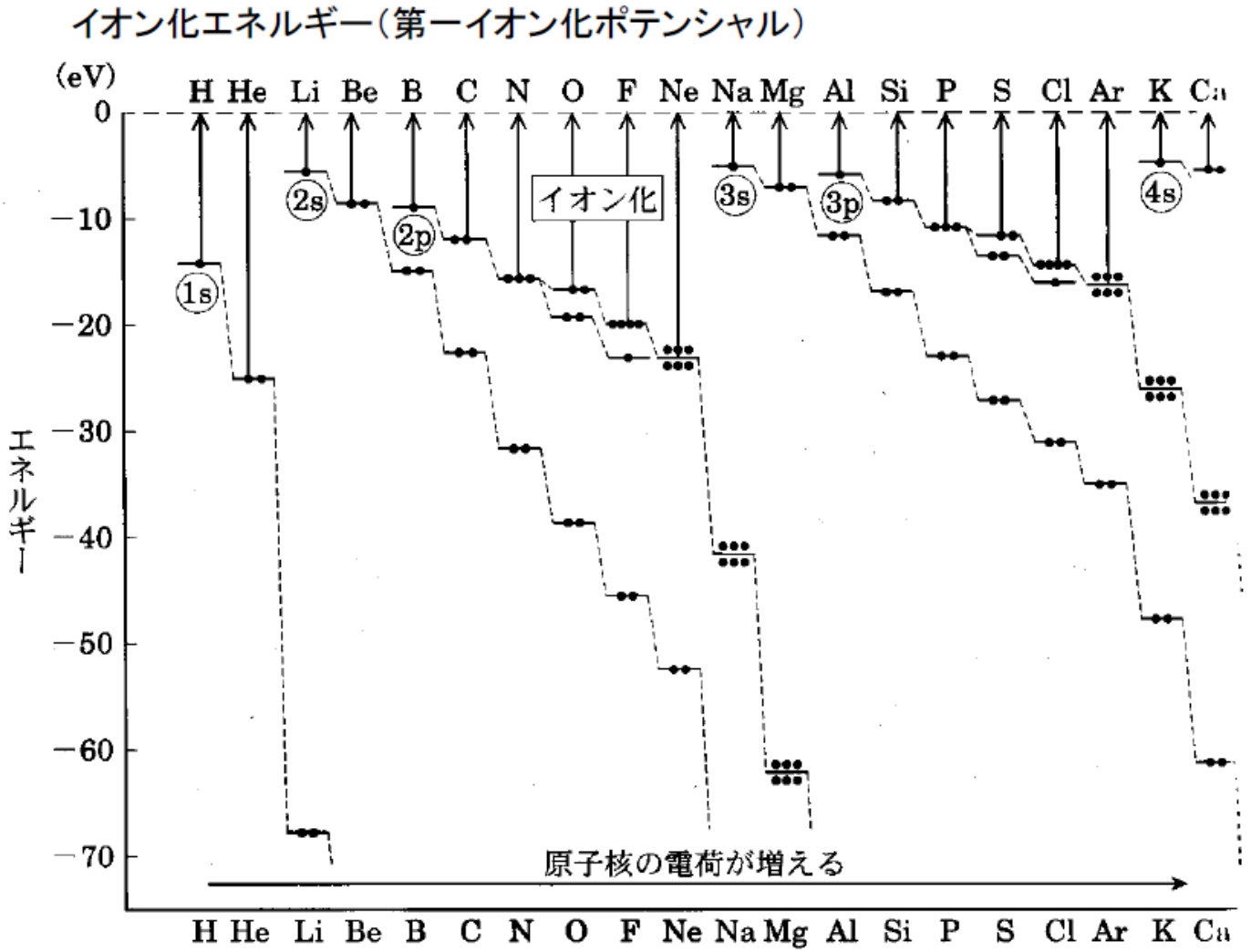
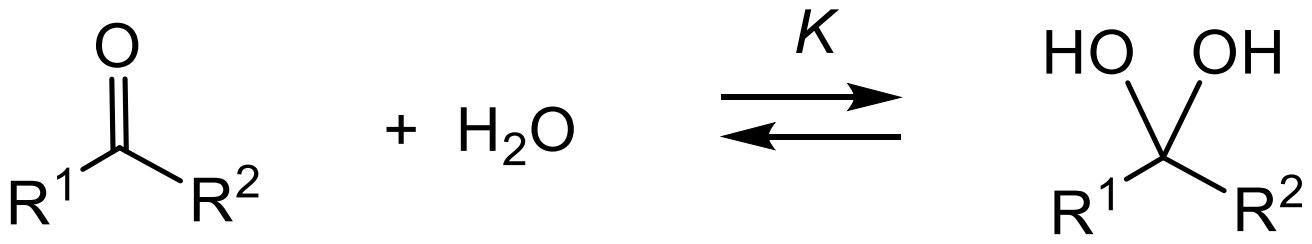
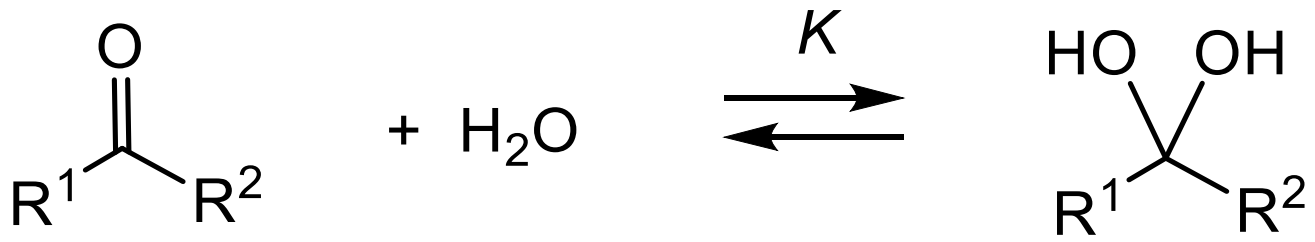



図6　水素（原子番号1）～カルシウム（20）の電子エネルギー準位（計算値）

# カルボニル化合物の水和について

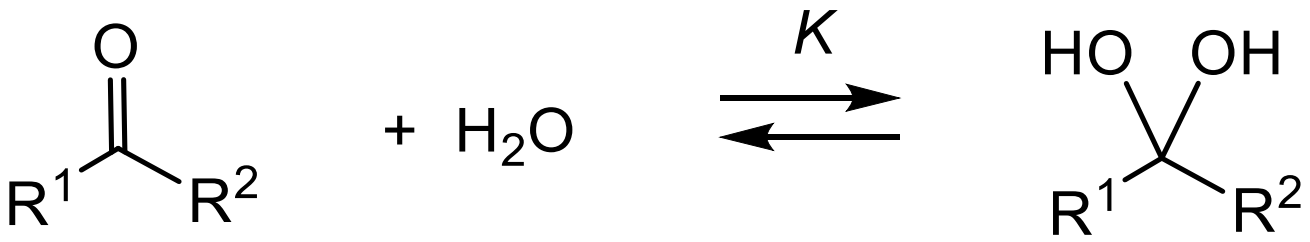


# カルボニル化合物の種類の影響




| $R^1$ | $R^2$ | rel. *K* | LUMO level (calc.) / eV | Partial charge on carbonyl carbon (calc.) | $\Delta H_f$ 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 |
| $CF_3$ | $CF_3$ | $1.2 \times 10^6$ | -1.5654 | +0.2882 | -340.02 |

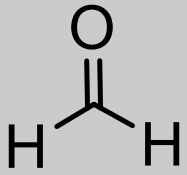
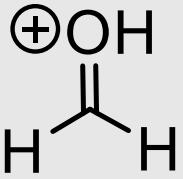
# カルボニル化合物の種類の影響(2)



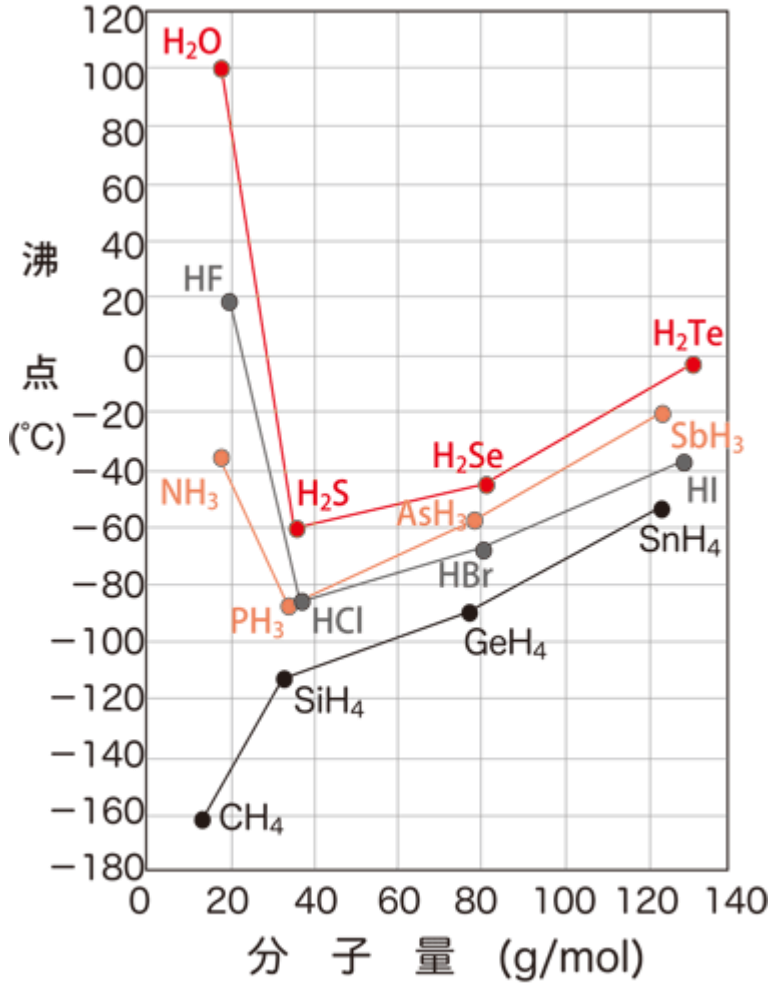

| $R^1$ | $R^2$ | rel. *K* | $\Delta H_f$(calc.) for C=O / *kcal mol*$^{-1}$ | $\Delta H_f$(calc.) for hydrate/ *kcal mol*$^{-1}$ | $\Delta H_r$(calc.) *kcal mol*$^{-1}$ |
|---|---|---|---|---|---|
| $CH_3$ | $CH_3$ | 0.001 | -52.98 | -115.57 | -62.59 |
| $CH_3$ | H | 1.06 | -44.19 | -107.97 | -63.78 |
| H | H | 2280 | -34.08 | -100.07 | -65.99 |
| $CCl_3$ | H | 2500 | -51.89 | -117.72 | -65.83 |
| $CF_3$ | $CF_3$ | $1.2 \times 10^6$ | -340.02 | -413.50 | -73.48 |

cf. $\Delta H_f$(calc.) for $H_2O$ = -53.42 *kcal mol*$^{-1}$

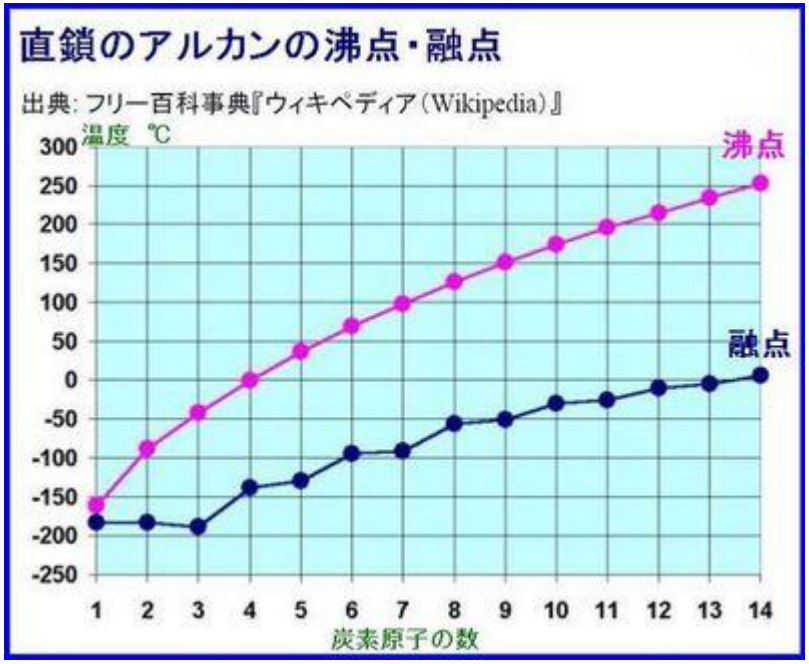
# 酸･塩基による反応加速

| species | Energy level (calc.)/ eV | Partial Charge (calc.) |
|---|---|---|
|  | 0.8266 (LUMO) | +0.2971 (C) |
|  | -7.8863 (LUMO) | +0.4718 (C) |
| $H_2O$ | -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




https://hyper-chemistry.blog.so-net.ne.jp/2010-03-27