# INPUT FORMAT FOR HUNDB

This guide created: June 10, 2002

| Line no. | Input | Format | Comments |
|---|---|---|---|
| 1 | TITEL | A5 | Name of molecule e.g. 'GeH' |
| 2 | NISO,IFLD,ISPEC,INTEN | * | NISO=number of isotopomers.<br>IFLD=0 for zero field calculations.<br>IFLD=1 for magnetic field calculations.<br>ISPEC=0 for a least-squares fit.<br>ISPEC=1 for spectrum prediction mode.<br>ISPEC=2 for plot of Zeeman splitting.<br>INTEN=0 no intensity calculation.<br>INTEN=1 for intensity calculation. |
| 3 | IMOD,IBOC | * | IMOD=0 for zero-point parameters ($B_0$, etc.)<br>IMOD=1 for equilibrium parameters ($B_e$, etc.)<br>IBOC : should always be set to 0<br>(= 1 for Born-Oppenheimer adiabatic corrections) |
| 4 | IDECOP,LABEL | * | IDECOP=0 for an **I**-decoupled basis set(LMR; $M_J, M_I$)<br>IDECOP=1 for a coupled basis set(zero-field; $M_F, F$)<br>LABEL=0 uses $J$ to indentify spin components<br>LABLE=1 uses $F_1 F_2$, etc. in increasing energy for given $J$ |
| 5 | XL | 14X,F5.1 | $\Lambda$ |
| 6 | XS | 14X,F5.1 | $S$ |
| 7 | XI | 14X,F5.1 | $I$ |
| 8 | UNIT | A3 | GHZ or CM-1 |

| Line no. | Input | Format | Parameters | Comments |
|---|---|---|---|---|
| 9 | P(1),P(2),P(41),P(42) | * | $\nu_0$ (or $\nu_e$), $\omega_e x_e$, B-O corr. | vibration |
| 10 | P(3),P(4) | * | $\omega_e y_e$, $\omega_e z_e$ | |
| 11 | P(5),P(6),P(45),P(46),P(57) | * | $B_0$, $\alpha_{\rm B}$, B-O corrections, $\beta_{\rm B}$ | rotation |
| 12 | P(7),P(8),P(58) | * | $D_0$, $\alpha_{\rm D}$, $\beta_{\rm D}$ | centrifugal distortion |
| 13 | P(9),P(10),P(59) | * | $\gamma_0$, $\alpha_\gamma$, $\beta_\gamma$ | spin-rotation |
| 14 | P(11),P(12) | * | $\lambda_0$, $\alpha_\lambda$ | spin-spin |
| 15 | P(13),P(14),P(60) | * | $A_0$, $\alpha_{\rm A}$, $\beta_{\rm A}$ | spin-orbit |
| 16 | P(15),P(16), | * | $\gamma_{\rm S}$, $\alpha_{\gamma_{\rm S}}$ | |
| 17 | P(75),P(76) | * | $\gamma_{\rm D}$, $\alpha_{\gamma_{\rm D}}$ | rot. correction to s-r |
| 18 | P(77),P(78) | * | $\lambda_{\rm D}$, $\alpha_{\lambda_{\rm D}}$ | rot. correction to s-s |
| 19 | P(79),P(80) | * | $H_0$, $\alpha_{\rm H}$ | $3^{\rm rd}$ order centrifugal distortion |
| 20 | P(17),P(18) | * | $p$, $\alpha_p$ | lambda doubling |
| 21 | P(19),P(20) | * | $q$, $\alpha_q$ | |
| 22 | P(63),P(64) | * | $p_{\rm D}$, $\alpha_{p_{\rm D}}$ | |
| 23 | P(65),P(66) | * | $q_{\rm D}$, $\alpha_{q_{\rm D}}$ | |
| 24 | P(21),P(22) | * | $q_\Delta$, $\alpha_{q_\Delta}$ | |
| 25 | P(23),P(24) | * | $p+4q$, $\alpha_{p+4q}$ | |
| 26 | P(25),P(26) | * | $a$, $\alpha_a$ | hyperfine |
| 27 | P(27),P(28) | * | $b_{\rm F}$, $\alpha_{b_{\rm F}}$ | |
| 28 | P(29),P(30) | * | $c$, $\alpha_c$ | |
| 29 | P(31),P(32) | * | $d$ ($C_{\rm I}$), $\alpha_d$ | |
| 30 | P(71),P(72) | * | $eq_0Q$, $\alpha_{\rm eq_0Q}$ | quadrupole |
| 31 | P(73),P(74) | * | $eq_2Q$, $\alpha_{\rm eq_2Q}$ | |
| 32 | P(33),P(34) | * | $g_{\rm s}$, $g_{\rm s}^v$ | Zeeman |
| 33 | P(35),P(36) | * | $g_{\rm L}$, $g_{\rm L}^v$ | |
| 34 | P(37),P(38) | * | $g_{\rm r}$, $g_{\rm r}^v$ | |
| 35 | P(39),P(40) | * | $g_{\rm l}$, $g_{\rm l}^v$ | |

| Line no. | Input | Format | Comments |
|---|---|---|---|
| 36 | IDN | * | $\Delta N$ for basis set |
| 37 | FLXC | * | Zeeman interpolation range (in Gauss) |
| 38 | DUMMY | A3 | ISO (lines in input file ignored until line beginning ISO) |
| 39 | A,B,XIIA | * | atomic mass of atoms A,B; nuclear spin of A, in isotopomer I |
| +I=1,NISO | | | |

| Line no. | Input | Format | Comments |
|---|---|---|---|
| | **ISPEC = 1 (prediction)**† | | |
| 40+NISO | DUMMY | A3 | CP+ (lines in input file ignored until line beginning CP+) |
| 41+NISO | INQUAD | * | ? |
| 42+NISO | ITERA | * | ? |
| 43+NISO | EPSB | * | ? |
| 44+NISO | DUMMY | A3 | DAT (lines in input file ignored until line beginning DAT) |
| 45+NISO | ISOT(I),XL2(I),VAU2(I), | * | isotope no., $\Lambda$, $v'$ |
| | XN2(I),XJ2(I), | | $N'$, $J'$ (LABEL=0) or spin-component label (LABEL=1) |
| | XHFS2(I),XM2(I) | | $M'_I$,$M'_J$ (IDECOP=0) or $F'$,$M'_F$ (IDECOP=1) |
| | IPAR2(I),FREQ(I) | | parity of upper state, transition frequency |
| +I=1,NDATA | | | |
| 46+NISO | XL1(I),VAU1(I), | * | $\Lambda$, $v$ |
| | XN1(I),XJ1(I), | | $N$, $J$ (LABEL=0) or spin-component label (LABEL=1) |
| | XHFS1(I),XM1(I) | | $M_I$,$M_J$ (IDECOP=0) or $F$,$M_F$ (IDECOP=1) |
| | IPAR1(I),FLUX(I),WT(I) | | parity of lower state, magnetic field, weight |
| +I=1,NDATA | | | |

† For zero-field (IFLD=0) omit lines 41-43, omit XMI(I), set FLUX(I) to 0

| Line no. | Input | Format | Comments |
|---|---|---|---|
| | **ISPEC = 2 (Zeeman plot)** | | |
| 40+NISO | DUMMY | A3 | CP+ or END (other lines ignored) |
| 41+NISO | INQUAD | * | =0,1 for linear,quadratic interpolation |
| 42+NISO | ITERA | * | No. iterations (up to 15) |
| 43+NISO | EPSB | * | tolerance limit of error in field |
| 44+NISO | DUMMY | A3 | CPL or end (other lines ignored) |
| 45+NISO | TTEXT | A80 | title to print at top of plot |
| 46+NISO | IKOINZ | * | =1 for pred. of laser line coincidences |
| 47+NISO | IOUT | * | ? |
| 48+NISO | IPLOT | * | =1 for Zeeman plot |
| 49+NISO | IPRED | * | =1 calls SPCALC to refine coincidences |
| 50+NISO | ISIM | * | =1 creates files for LMRSIM |
| 51+NISO | CPOL | A1 | =S,P,3,4 for $\sigma$-pol., $\pi$-pol. |
| 52+NISO | IUD | * | =3,4 for plot on screen, creation of ps file |
| 53+NISO | FPLOT | * | laser freq. for plot (=PLASER) |
| 54+NISO | DUMMY | A3 | DAT or END (other lines ignored) |
| 55+NISO | ISO,XL2,VAU2, | * | isotope no., $\Lambda$, $v'$ |
| | XN2,XJ2, | | $N'$, $J'$ (LABEL=0) or spin-component label (LABEL=1) |
| | XHFS2 | | $M_I'$ (IDECOP=0) or $F'$ (IDECOP=1) |
| | IPAR2,NFREQ | | parity of upper state, transition frequency |
| | NEUPIC,BMIN,PLTMIN | | starts new Zeeman plot if =1, min field (G), min freq |
| +I=1,NDATA | | | |
| 56+NISO | XL1,VAU1, | * | isotope no., $\Lambda$, $v$ |
| | XN1,XJ1, | | $N$, $J$ (LABEL=0) or spin-component label (LABEL=1) |
| | XHFS1 | | $M_I$ (IDECOP=0) or $F$ (IDECOP=1) |
| | IPAR1,NOFLD, | | parity of upper state, no. iterations to refine field (up to 15) |
| | IAUTO,BMAX,PLTMAX | | automatic scaling of plots if =1, max field (G), max freq |
| 57+ISO | PLASER | * | frequency of laser line |
| I=1,NFREQ | | | |

| Line no. | Input | Format | Comments |
|---|---|---|---|
| | **ISPEC = 0 (fit)**[†] | | |
| 40+NISO | DUMMY | A3 | CFI (lines in input file ignored until line beginning CFI) |
| 41+NISO | NDATA,NFLOAT,ITRN, | 3I4 | no. data points, floated parameters, fit iterations |
| | TST, | F10.3 | if fractional change in std. dev. $\leq$ TST, terminate fit |
| | IWU | I4 | IWU=1 uses uncertainties, IWU=0 uses weights |
| 42+NISO | PP(I), I=1,NCONS(80) | 80I1 | PP(I)=1 to float P(I) in fit, NCONS set to 80 |
| 43+NISO | DUMMY | A3 | DAT (lines in input file ignored until line beginning DAT) |
| 44+NISO | ISOT(I),XL2(I),VAU2(I), | * | isotope no., $\Lambda$, $v'$ |
| | XN2(I),XJ2(I), | | $N'$, $J'$ (LABEL=0) or spin-component label (LABEL=1) |
| | XHFS2(I),XM2(I) | | $M_I'$,$M_J'$ (IDECOP=0) or $F'$,$M_F'$ (IDECOP=1) |
| | IPAR2(I),FREQ(I) | | parity of upper state, transition frequency |
| +I=1,NDATA | | | |
| 45+NISO | XL1(I),VAU1(I), | * | $\Lambda$, $v$ |
| | XN1(I),XJ1(I), | | $N$, $J$ (LABEL=0) or spin-component label (LABEL=1) |
| | XHFS1(I),XM1(I) | | $M_I$,$M_J$ (IDECOP=0) or $F$,$M_F$ (IDECOP=1) |
| | IPAR1(I),FLUX(I),WT(I) | | parity of lower state, magnetic field, weight |
| +I=1,NDATA | | | |

[†] For IFLD=0 omit XM1(I), XM2(I) and set FLUX(I) to 0