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ON THE CALCULATION OF LANTHANIDE SYSTEMS. THE SPECTRAL PARAMETERS OF PRASEODYMIUM TRIVALENT ION

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The following data are serving to the treatment outlined in the main text, expressing the spectral terms from f^2 and *fd* configurations in terms of the Slater-Condon integrals. The strategy is a shortcut based only on the evaluation of the diagonal matrix elements of a poly-electronic Hamiltonian. In a basis of Slater determinants, Ω_P, the diagonal elements [Slater J (1929) "The theory of complex spectra". *Phys. Rev.* 1929, 34:1293–1322, Slater J "Analytic atomic wave functions." *Phys. Rev.* 1932, 42:33-43] are expressed as Eq.(S1).

$$\langle \Omega_P | \hat{H} | \Omega_P \rangle = \sum_{a \in P} h_{aa} + \sum_{a \in P} \sum_{b<a} [(ab|ab) - (ab|ba)] \quad , \tag{S1}$$

where, *a* and *b* are spin-orbitals entering in the composition of the given Slater determinant. The *h* denotes the one-electron Hamiltonian component (electron-nuclear term plus kinetic energy of one electron, labeled 1):

$$h_{aa} = \int a^*(1) \hat{h}\, a(1) d\boldsymbol{V}_1. \tag{S2}$$

The (*ab*|*ab*) and (*ab*|*ba*) denote the Coulomb and exchange two-electron integrals:

$$(ab|ab) = \int_{V_1} \int_{V_2} a^*(1) b^*(2) \frac{1}{r_{12}}\, a(1) b(2) d\boldsymbol{V}_1 d\boldsymbol{V}_2 \ , \tag{S3}$$

$$(ab|ba) = \int_{V_1} \int_{V_2} a^*(1) b^*(2) \frac{1}{r_{12}}\, b(1) a(2) d\boldsymbol{V}_1 d\boldsymbol{V}_2 \ . \tag{S4}$$

For the analysis given in the main text, it is convenient to work with complex atomic orbitals, labeled by the l_z projections of the secondary quantum number *l*, with $l_z \in \{-l, \ldots 0, \ldots, l\}$. The Tables S1 and S2 are giving the two-electron integrals needed to apply the (S1) equation in the case of general configurations with *f* and *d* orbitals. The l_z projections are ascribed as subscripts to the shell label. Note the general equivalence (*ab*|*ab*)= (*ba*|*ba*) and (*ab*|*ba*)= (*ba*|*ab*)= (*aa*|*bb*) = (*bb*|*aa*).

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Table S1

Two electron integrals made with *f*-type orbitals, as function of F_k^{ff} Slater-Condon parameters.

Formulas	*Integrals*
$F_0^{ff} + 16F_2^{ff} + 36F_4^{ff} + 400F_6^{ff}$	$(f_0f_0\|f_0f_0)$
$F_0^{ff} + 9F_2^{ff} + F_4^{ff} + 225F_6^{ff}$	$(f_1f_1\|f_1f_1)$, $(f_1f_{-1}\|f_1f_{-1})$, $(f_{-1}f_1\|f_{-1}f_1)$, $(f_{-1}f_{-1}\|f_{-1}f_{-1})$
$F_0^{ff} + 49F_4^{ff} + 36F_6^{ff}$	$(f_2f_2\|f_2f_2)$, $(f_2f_{-2}\|f_2f_{-2})$, $(f_{-2}f_2\|f_{-2}f_2)$, $(f_{-2}f_{-2}\|f_{-2}f_{-2})$
$F_0^{ff} + 25F_2^{ff} + 9F_4^{ff} + F_6^{ff}$	$(f_3f_{-3}\|f_3f_{-3})$, $(f_{-3}f_3\|f_{-3}f_3)$, $(f_{-3}f_{-3}\|f_{-3}f_{-3})$, $(f_3f_3\|f_3f_3)$
$F_0^{ff} + 12F_2^{ff} + 6F_4^{ff} - 300F_6^{ff}$	$f_0f_1\|f_0f_1)$, $(f_0f_{-1}\|f_0f_{-1})$, $(f_1f_0\|f_1f_0)$, $(f_{-1}f_0\|f_{-1}f_0)$
$F_0^{ff} - 42F_4^{ff} + 120F_6^{ff}$	$(f_0f_2\|f_0f_2)$, $(f_0f_{-2}\|f_0f_{-2})$, $(f_2f_0\|f_2f_0)$, $(f_{-2}f_0\|f_{-2}f_0)$
$F_0^{ff} - 7F_4^{ff} - 90F_6^{ff}$	$(f_1f_2\|f_1f_2)$, $(f_1f_{-2}\|f_1f_{-2})$, $(f_{-1}f_2\|f_{-1}f_2)$, $(f_{-1}f_{-2}\|f_{-1}f_{-2})$, $(f_2f_1\|f_2f_1)$, $(f_2f_{-1}\|f_2f_{-1})$, $(f_{-2}f_1\|f_{-2}f_1)$, $(f_{-2}f_{-1}\|f_{-2}f_{-1})$
$F_0^{ff} - 15F_2^{ff} + 3F_4^{ff} + 15F_6^{ff}$	$(f_1f_3\|f_1f_3)$, $(f_1f_{-3}\|f_1f_{-3})$, $(f_{-1}f_3\|f_{-1}f_3)$, $(f_{-1}f_{-3}\|f_{-1}f_{-3})$, $(f_3f_1\|f_3f_1)$, $(f_3f_{-1}\|f_3f_{-1})$, $(f_{-3}f_1\|f_{-3}f_1)$, $(f_{-3}f_{-1}\|f_{-3}f_{-1})$
$F_0^{ff} - 20F_2^{ff} + 18F_4^{ff} - 20F_6^{ff}$	$(f_0f_3\|f_0f_3)$, $(f_0f_{-3}\|f_0f_{-3})$, $(f_3f_0\|f_3f_0)$, $(f_{-3}f_0\|f_{-3}f_0)$
$F_0^{ff} - 21F_4^{ff} - 6F_6^{ff}$	$(f_2f_3\|f_2f_3)$, $(f_2f_{-3}\|f_2f_{-3})$, $(f_{-2}f_3\|f_{-2}f_3)$, $(f_{-2}f_{-3}\|f_{-2}f_{-3})$, $(f_3f_2\|f_3f_2)$, $(f_3f_{-2}\|f_3f_{-2})$, $(f_{-3}f_2\|f_{-3}f_2)$, $(f_{-3}f_{-2}\|f_{-3}f_{-2})$
$10F_2^{ff} + 54F_4^{ff} + 28F_6^{ff}$	$(f_1f_{-1}\|f_3f_{-3})$, $(f_{-1}f_1\|f_{-3}f_3)$, $(f_1f_3\|f_3f_1)$, $(f_{-1}f_{-3}\|f_{-3}f_{-1})$, $(f_3f_1\|f_1f_3)$, $(f_{-3}f_{-1}\|f_{-1}f_{-3})$, $(f_3f_{-3}\|f_1f_{-1})$, $(f_{-3}f_3\|f_{-1}f_1)$
$14F_4^{ff} + 378F_6^{ff}$	$(f_1f_{-2}\|f_{-2}f_1)$, $(f_{-1}f_2\|f_2f_{-1})$, $(f_2f_{-1}\|f_{-1}f_2)$, $(f_{-2}f_1\|f_1f_{-2})$
$-14F_4^{ff} - 378F_6^{ff}$	$(f_1f_{-1}\|f_{-2}f_2)$, $(f_{-1}f_1\|f_2f_{-2})$, $(f_2f_{-2}\|f_{-1}f_1)$, $(f_{-2}f_2\|f_1f_{-1})$
$15F_2^{ff} + 32F_4^{ff} + 105F_6^{ff}$	$(f_1f_2\|f_2f_1)$, $(f_{-1}f_{-2}\|f_{-2}f_{-1})$, $(f_2f_1\|f_1f_2)$, $(f_{-2}f_{-1}\|f_{-1}f_{-2})$
$-15F_2^{ff} - 32F_4^{ff} - 105F_6^{ff}$	$(f_1f_{-1}\|f_2f_{-2})$, $(f_{-1}f_1\|f_{-2}f_2)$, $(f_2f_{-2}\|f_1f_{-1})$, $(f_{-2}f_2\|f_{-1}f_1)$
$20F_2^{ff} + 3F_4^{ff} + 224F_6^{ff}$	$(f_0f_0\|f_2f_{-2})$, $(f_0f_0\|f_{-2}f_2)$, $(f_0f_2\|f_2f_0)$, $(f_0f_{-2}\|f_{-2}f_0)$, $(f_2f_0\|f_0f_2)$, $(f_{-2}f_0\|f_0f_{-2})$, $(f_2f_{-2}\|f_0f_0)$, $(f_{-2}f_2\|f_0f_0)$
$20F_2^{ff} + 3F_4^{ff} + 224F_6^{ff}$	$(f_0f_0\|f_2f_{-2})$, $(f_0f_0\|f_{-2}f_2)$, $(f_0f_2\|f_2f_0)$, $(f_0f_{-2}\|f_{-2}f_0)$, $(f_2f_0\|f_0f_2)$, $(f_{-2}f_0\|f_0f_{-2})$, $(f_2f_{-2}\|f_0f_0)$, $(f_{-2}f_2\|f_0f_0)$
$20F_2^{ff} + 3F_4^{ff} + 224F_6^{ff}$	$(f_0f_0\|f_2f_{-2})$, $(f_0f_0\|f_{-2}f_2)$, $(f_0f_2\|f_2f_0)$, $(f_0f_{-2}\|f_{-2}f_0)$, $(f_2f_0\|f_0f_2)$, $(f_{-2}f_0\|f_0f_{-2})$, $(f_2f_{-2}\|f_0f_0)$, $(f_{-2}f_2\|f_0f_0)$
$24F_2^{ff} + 40F_4^{ff} + 420F_6^{ff}$	$(f_1f_{-1}\|f_{-1}f_1)$, $(f_{-1}f_1\|f_1f_{-1})$
$25F_2^{ff} + 30F_4^{ff} + 7F_6^{ff}$	$(f_2f_3\|f_3f_2)$, $(f_{-2}f_{-3}\|f_{-3}f_{-2})$, $(f_3f_2\|f_2f_3)$, $(f_{-3}f_{-2}\|f_{-2}f_{-3})$
$-25F_2^{ff} - 30F_4^{ff} - 7F_6^{ff}$	$(f_2f_{-2}\|f_3f_{-3})$, $(f_{-2}f_2\|f_{-3}f_3)$, $(f_3f_{-3}\|f_2f_{-2})$, $(f_{-3}f_3\|f_{-2}f_2)$
$2F_2^{ff} + 15F_4^{ff} + 350F_6^{ff}$	$(f_0f_1\|f_1f_0)$, $(f_0f_{-1}\|f_{-1}f_0)$, $(f_1f_0\|f_0f_1)$, $(f_{-1}f_0\|f_0f_{-1})$
$-2F_2^{ff} - 15F_4^{ff} - 350F_6^{ff}$	$(f_0f_0\|f_1f_{-1})$, $(f_0f_0\|f_{-1}f_1)$, $(f_1f_{-1}\|f_0f_0)$, $(f_{-1}f_1\|f_0f_0)$
$42F_4^{ff} + 210F_6^{ff}$	$(f_1f_{-1}\|f_{-3}f_3)$, $(f_{-1}f_1\|f_3f_{-3})$, $(f_1f_{-3}\|f_{-3}f_1)$, $(f_{-1}f_3\|f_3f_{-1})$, $(f_3f_{-1}\|f_{-1}f_3)$, $(f_{-3}f_1\|f_1f_{-3})$, $(f_3f_{-3}\|f_{-1}f_1)$, $(f_{-3}f_3\|f_1f_{-1})$
$462F_6^{ff}$	$(f_2f_{-3}\|f_{-3}f_2)$, $(f_{-2}f_3\|f_3f_{-2})$, $(f_3f_{-2}\|f_{-2}f_3)$, $(f_{-3}f_2\|f_2f_{-3})$
$-462F_6^{ff}$	$(f_2f_{-2}\|f_{-3}f_3)$, $(f_{-2}f_2\|f_3f_{-3})$, $(f_3f_{-3}\|f_{-2}f_2)$, $(f_{-3}f_3\|f_2f_{-2})$
$63F_4^{ff} + 84F_6^{ff}$	$(f_0f_3\|f_3f_0)$, $(f_0f_{-3}\|f_{-3}f_0)$, $(f_3f_0\|f_0f_3)$, $(f_{-3}f_0\|f_0f_{-3})$
$-63F_4^{ff} - 84F_6^{ff}$	$(f_0f_0\|f_3f_{-3})$, $(f_0f_0\|f_{-3}f_3)$, $(f_3f_{-3}\|f_0f_0)$, $(f_{-3}f_3\|f_0f_0)$
$70F_4^{ff} + 504F_6^{ff}$	$(f_2f_{-2}\|f_{-2}f_2)$, $(f_{-2}f_2\|f_2f_{-2})$
$924F_6^{ff}$	$(f_3f_{-3}\|f_{-3}f_3)$, $(f_{-3}f_3\|f_3f_{-3})$

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Table S2

Two electron integrals between *f*- and *d* orbitals, as function of F_k^{fd} and G_k^{fd} Slater-Condon parameters.

Formulas	*Integrals*
$F_0^{fd} + 10F_2^{fd} + 3F_4^{fd}$	$(d_{-2}f_{-3} \mid d_{-2}f_{-3})$, $(d_2f_{-3} \mid d_2f_{-3})$, $(d_{-2}f_3 \mid d_{-2}f_3)$, $(d_2f_3 \mid d_2f_3)$, $(f_{-3}d_{-2} \mid f_{-3}d_{-2})$, $(f_3d_{-2} \mid f_3d_{-2})$, $(f_{-3}d_2 \mid f_{-3}d_2)$, $(f_3d_2 \mid f_3d_2)$
$F_0^{fd} + 28F_4^{fd}$	$(d_{-1}f_{-2} \mid d_{-1}f_{-2})$, $(d_1f_{-2} \mid d_1f_{-2})$, $(d_{-1}f_2 \mid d_{-1}f_2)$, $(d_1f_2 \mid d_1f_2)$, $(f_{-2}d_{-1} \mid f_{-2}d_{-1})$, $(f_2d_{-1} \mid f_2d_{-1})$, $(f_{-2}d_1 \mid f_{-2}d_1)$, $(f_2d_1 \mid f_2d_1)$
$F_0^{fd} + 3F_2^{fd} - 4F_4^{fd}$	$(d_{-1}f_{-1} \mid d_{-1}f_{-1})$, $(d_1f_{-1} \mid d_1f_{-1})$, $(d_{-1}f_1 \mid d_{-1}f_1)$, $(d_1f_1 \mid d_1f_1)$, $(f_{-1}d_{-1} \mid f_{-1}d_{-1})$, $(f_1d_{-1} \mid f_1d_{-1})$, $(f_{-1}d_1 \mid f_{-1}d_1)$, $(f_1d_1 \mid f_1d_1)$
$F_0^{fd} + 4F_2^{fd} - 24F_4^{fd}$	$(d_{-1}f_0 \mid d_{-1}f_0)$, $(d_1f_0 \mid d_1f_0)$, $(f_0d_{-1} \mid f_0d_{-1})$, $(f_0d_1 \mid f_0d_1)$
$F_0^{fd} + 6F_2^{fd} + 6F_4^{fd}$	$(d_0f_{-1} \mid d_0f_{-1})$, $(d_0f_1 \mid d_0f_1)$, $(f_{-1}d_0 \mid f_{-1}d_0)$, $(f_1d_0 \mid f_1d_0)$
$F_0^{fd} + 8F_2^{fd} + 36F_4^{fd}$	$(d_0f_0 \mid d_0f_0)$, $(f_0d_0 \mid f_0d_0)$
$F_0^{fd} - 10F_2^{fd} + 18F_4^{fd}$	$(d_0f_{-3} \mid d_0f_{-3})$, $(d_0f_3 \mid d_0f_3)$, $(f_{-3}d_0 \mid f_{-3}d_0)$, $(f_3d_0 \mid f_3d_0)$
$F_0^{fd} - 42F_4^{fd}$	$(d_0f_{-2} \mid d_0f_{-2})$, $(d_0f_2 \mid d_0f_2)$, $(f_{-2}d_0 \mid f_{-2}d_0)$, $(f_2d_0 \mid f_2d_0)$
$F_0^{fd} - 5F_2^{fd} - 12F_4^{fd}$	$(d_{-1}f_{-3} \mid d_{-1}f_{-3})$, $(d_1f_{-3} \mid d_1f_{-3})$, $(d_{-1}f_3 \mid d_{-1}f_3)$, $(d_1f_3 \mid d_1f_3)$, $(f_{-3}d_{-1} \mid f_{-3}d_{-1})$, $(f_3d_{-1} \mid f_3d_{-1})$, $(f_{-3}d_1 \mid f_{-3}d_1)$, $(f_3d_1 \mid f_3d_1)$
$F_0^{fd} - 6F_2^{fd} + F_4^{fd}$	$(d_{-2}f_{-1} \mid d_{-2}f_{-1})$, $(d_2f_{-1} \mid d_2f_{-1})$, $(d_{-2}f_1 \mid d_{-2}f_1)$, $(d_2f_1 \mid d_2f_1)$, $(f_{-1}d_{-2} \mid f_{-1}d_{-2})$, $(f_1d_{-2} \mid f_1d_{-2})$, $(f_{-1}d_2 \mid f_{-1}d_2)$, $(f_1d_2 \mid f_1d_2)$
$F_0^{fd} - 7F_4^{fd}$	$(d_{-2}f_{-2} \mid d_{-2}f_{-2})$, $(d_2f_{-2} \mid d_2f_{-2})$, $(d_{-2}f_2 \mid d_{-2}f_2)$, $(d_2f_2 \mid d_2f_2)$, $(f_{-2}d_{-2} \mid f_{-2}d_{-2})$, $(f_2d_{-2} \mid f_2d_{-2})$, $(f_{-2}d_2 \mid f_{-2}d_2)$, $(f_2d_2 \mid f_2d_2)$
$F_0^{fd} - 8F_2^{fd} + 6F_4^{fd}$	$(d_{-2}f_0 \mid d_{-2}f_0)$, $(d_2f_0 \mid d_2f_0)$, $(f_0d_{-2} \mid f_0d_{-2})$, $(f_0d_2 \mid f_0d_2)$
$12F_2^{fd} + 40F_4^{fd}$	$(d_1f_{-1} \mid d_{-1}f_1)$, $(d_{-1}f_1 \mid d_1f_{-1})$, $(f_1d_{-1} \mid f_{-1}d_1)$, $(f_{-1}d_1 \mid f_1d_{-1})$
$70F_4^{fd}$	$(d_2f_{-2} \mid d_{-2}f_2)$, $(d_{-2}f_2 \mid d_2f_{-2})$, $(f_2d_{-2} \mid f_{-2}d_2)$, $(f_{-2}d_2 \mid f_2d_{-2})$
$10G_1^{fd} + 15G_3^{fd} + 24G_5^{fd}$	$(d_{-1}f_{-2} \mid f_{-2}d_{-1})$, $(d_1f_2 \mid f_2d_1)$, $(f_{-2}d_{-1} \mid d_{-1}f_{-2})$, $(f_2d_1 \mid d_1f_2)$
$-10G_1^{fd} - 15G_3^{fd} - 24G_5^{fd}$	$(d_1d_{-1} \mid f_2f_{-2})$, $(d_{-1}d_1 \mid f_{-2}f_2)$, $(f_2f_{-2} \mid d_1d_{-1})$, $(f_{-2}f_2 \mid d_{-1}d_1)$
$10G_3^{fd} + 70G_5^{fd}$	$(d_2f_{-1} \mid f_{-1}d_2)$, $(d_{-2}f_1 \mid f_1d_{-2})$, $(f_1d_{-2} \mid d_{-2}f_1)$, $(f_{-1}d_2 \mid d_2f_{-1})$
$-10G_3^{fd} - 70G_5^{fd}$	$(d_2d_{-2} \mid f_{-1}f_1)$, $(d_{-2}d_2 \mid f_1f_{-1})$, $(f_1f_{-1} \mid d_{-2}d_2)$, $(f_{-1}f_1 \mid d_2d_{-2})$
$126G_5^{fd}$	$(d_2d_{-2} \mid f_{-2}f_2)$, $(d_{-2}d_2 \mid f_2f_{-2})$, $(d_2f_{-2} \mid f_{-2}d_2)$, $(d_{-2}f_2 \mid f_2d_{-2})$, $(f_2d_{-2} \mid d_{-2}f_2)$, $(f_{-2}d_2 \mid d_2f_{-2})$, $(f_2f_{-2} \mid d_{-2}d_2)$, $(f_{-2}f_2 \mid d_2d_{-2})$
$15G_1^{fd} + 10G_3^{fd} + G_5^{fd}$	$(d_{-2}f_{-3} \mid f_{-3}d_{-2})$, $(d_2f_3 \mid f_3d_2)$, $(f_{-3}d_{-2} \mid d_{-2}f_{-3})$, $(f_3d_2 \mid d_2f_3)$
$-15G_1^{fd} - 10G_3^{fd} - G_5^{fd}$	$(d_2d_{-2} \mid f_3f_{-3})$, $(d_{-2}d_2 \mid f_{-3}f_3)$, $(f_3f_{-3} \mid d_2d_{-2})$, $(f_{-3}f_3 \mid d_{-2}d_2)$
$15G_3^{fd} + 105G_5^{fd}$	$(d_1d_{-1} \mid f_{-1}f_1)$, $(d_{-1}d_1 \mid f_1f_{-1})$, $(d_1f_{-1} \mid f_{-1}d_1)$, $(d_{-1}f_1 \mid f_1d_{-1})$, $(f_1d_{-1} \mid d_{-1}f_1)$, $(f_{-1}d_1 \mid d_1f_{-1})$, $(f_1f_{-1} \mid d_{-1}d_1)$, $(f_{-1}f_1 \mid d_1d_{-1})$
$20G_3^{fd} + 35G_5^{fd}$	$(d_2d_{-2} \mid f_0f_0)$, $(d_{-2}d_2 \mid f_0f_0)$, $(d_{-2}f_0 \mid f_0d_{-2})$, $(d_2f_0 \mid f_0d_2)$, $(f_0d_{-2} \mid d_{-2}f_0)$, $(f_0d_2 \mid d_2f_0)$, $(f_0f_0 \mid d_2d_{-2})$, $(f_0f_0 \mid d_{-2}d_2)$
$210G_5^{fd}$	$(d_2f_{-3} \mid f_{-3}d_2)$, $(d_{-2}f_3 \mid f_3d_{-2})$, $(f_3d_{-2} \mid d_{-2}f_3)$, $(f_{-3}d_2 \mid d_2f_{-3})$
$-210G_5^{fd}$	$(d_2d_{-2} \mid f_{-3}f_3)$, $(d_{-2}d_2 \mid f_3f_{-3})$, $(f_3f_{-3} \mid d_{-2}d_2)$, $(f_{-3}f_3 \mid d_2d_{-2})$
$25G_3^{fd} + 112G_5^{fd}$	$(d_1f_{-2} \mid f_{-2}d_1)$, $(d_{-1}f_2 \mid f_2d_{-1})$, $(f_2d_{-1} \mid d_{-1}f_2)$, $(f_{-2}d_1 \mid d_1f_{-2})$
$25G_3^{fd} + 28G_5^{fd}$	$(d_0f_{-3} \mid f_{-3}d_0)$, $(d_0f_3 \mid f_3d_0)$, $(f_{-3}d_0 \mid d_0f_{-3})$, $(f_3d_0 \mid d_0f_3)$
$25G_3^{fd} + 7G_5^{fd}$	$(d_1d_{-1} \mid f_3f_{-3})$, $(d_{-1}d_1 \mid f_{-3}f_3)$, $(d_{-1}f_{-3} \mid f_{-3}d_{-1})$, $(d_1f_3 \mid f_3d_1)$, $(f_{-3}d_{-1} \mid d_{-1}f_{-3})$, $(f_3d_1 \mid d_1f_3)$, $(f_3f_{-3} \mid d_1d_{-1})$, $(f_{-3}f_3 \mid d_{-1}d_1)$
$-25G_3^{fd} - 112G_5^{fd}$	$(d_1d_{-1} \mid f_{-2}f_2)$, $(d_{-1}d_1 \mid f_2f_{-2})$, $(f_2f_{-2} \mid d_{-1}d_1)$, $(f_{-2}f_2 \mid d_1d_{-1})$
$-25G_3^{fd} - 28G_5^{fd}$	$(d_0d_0 \mid f_3f_{-3})$, $(d_0d_0 \mid f_{-3}f_3)$, $(f_3f_{-3} \mid d_0d_0)$, $(f_{-3}f_3 \mid d_0d_0)$
$3G_1^{fd} + 2G_3^{fd} + 80G_5^{fd}$	$(d_{-1}f_0 \mid f_0d_{-1})$, $(d_1f_0 \mid f_0d_1)$, $(f_0d_{-1} \mid d_{-1}f_0)$, $(f_0d_1 \mid d_1f_0)$

	$-3G_1^{fd} - 2G_3^{fd} - 80G_5^{fd}$	$(d_1d_{-1} \mid f_0f_0)$, $(d_{-1}d_1 \mid f_0f_0)$, $(f_0f_0 \mid d_1d_{-1})$, $(f_0f_0 \mid d_{-1}d_1)$
	$5G_1^{fd} + 20G_3^{fd} + 5G_5^{fd}$	$(d_{-2}d_{-2} \mid f_{-2}f_{-2})$, $(d_2d_{-2} \mid f_2f_{-2})$, $(d_{-2}d_2 \mid f_{-2}f_2)$, $(d_2d_2 \mid f_2f_2)$, $(d_{-2}f_{-2} \mid f_{-2}d_{-2})$, $(d_2f_{-2} \mid f_2d_{-2})$, $(d_{-2}f_2 \mid f_{-2}d_2)$, $(d_2f_2 \mid f_2d_2)$, $(f_{-2}d_{-2} \mid d_{-2}f_{-2})$, $(f_2d_{-2} \mid d_2f_{-2})$, $(f_{-2}d_2 \mid d_{-2}f_2)$, $(f_2d_2 \mid d_2f_2)$, $(f_{-2}f_{-2} \mid d_{-2}d_{-2})$, $(f_2f_{-2} \mid d_2d_{-2})$, $(f_{-2}f_2 \mid d_{-2}d_2)$, $(f_2f_2 \mid d_2d_2)$
	$63G_5^{fd}$	$(d_0d_0 \mid f_2f_{-2})$, $(d_0d_0 \mid f_{-2}f_2)$, $(d_0f_{-2} \mid f_{-2}d_0)$, $(d_0f_2 \mid f_2d_0)$, $(f_{-2}d_0 \mid d_0f_{-2})$, $(f_2d_0 \mid d_0f_2)$, $(f_2f_{-2} \mid d_0d_0)$, $(f_{-2}f_2 \mid d_0d_0)$
	$6G_1^{fd} + 9G_3^{fd} + 90G_5^{fd}$	$(d_0f_{-1} \mid f_{-1}d_0)$, $(d_0f_1 \mid f_1d_0)$, $(f_{-1}d_0 \mid d_0f_{-1})$, $(f_1d_0 \mid d_0f_1)$
	$-6G_1^{fd} - 9G_3^{fd} - 90G_5^{fd}$	$(d_0d_0 \mid f_1f_{-1})$, $(d_0d_0 \mid f_{-1}f_1)$, $(f_1f_{-1} \mid d_0d_0)$, $(f_{-1}f_1 \mid d_0d_0)$
$84G_5^{fd}$		$(d_1d_{-1} \mid f_{-3}f_3)$, $(d_{-1}d_1 \mid f_3f_{-3})$, $(d_1f_{-3} \mid f_{-3}d_1)$, $(d_{-1}f_3 \mid f_3d_{-1})$, $(f_3d_{-1} \mid d_{-1}f_3)$, $(f_{-3}d_1 \mid d_1f_{-3})$, $(f_3f_{-3} \mid d_{-1}d_1)$, $(f_{-3}f_3 \mid d_1d_{-1})$
	$8G_1^{fd} + 2G_3^{fd} + 50G_5^{fd}$	$(d_{-1}d_{-1} \mid f_{-1}f_{-1})$, $(d_1d_{-1} \mid f_1f_{-1})$, $(d_{-1}d_1 \mid f_{-1}f_1)$, $(d_1d_1 \mid f_1f_1)$, $(d_{-1}f_{-1} \mid f_{-1}d_{-1})$, $(d_1f_{-1} \mid f_1d_{-1})$, $(d_{-1}f_1 \mid f_{-1}d_1)$, $(d_1f_1 \mid f_1d_1)$, $(f_{-1}d_{-1} \mid d_{-1}f_{-1})$, $(f_1d_{-1} \mid d_1f_{-1})$, $(f_{-1}d_1 \mid d_{-1}f_1)$, $(f_1d_1 \mid d_1f_1)$, $(f_{-1}f_{-1} \mid d_{-1}d_{-1})$, $(f_1f_{-1} \mid d_1d_{-1})$, $(f_{-1}f_1 \mid d_{-1}d_1)$, $(f_1f_1 \mid d_1d_1)$
	$9G_1^{fd} + 16G_3^{fd} + 100G_5^{fd}$	$(d_0d_0 \mid f_0f_0)$, $(d_0f_0 \mid f_0d_0)$, $(f_0d_0 \mid d_0f_0)$, $(f_0f_0 \mid d_0d_0)$
	$G_1^{fd} + 24G_3^{fd} + 15G_5^{fd}$	$(d_{-2}f_{-1} \mid f_{-1}d_{-2})$, $(d_2f_1 \mid f_1d_2)$, $(f_{-1}d_{-2} \mid d_{-2}f_{-1})$, $(f_1d_2 \mid d_2f_1)$
	$-G_1^{fd} - 24G_3^{fd} - 15G_5^{fd}$	$(d_2d_{-2} \mid f_1f_{-1})$, $(d_{-2}d_2 \mid f_{-1}f_1)$, $(f_1f_{-1} \mid d_2d_{-2})$, $(f_{-1}f_1 \mid d_{-2}d_2)$

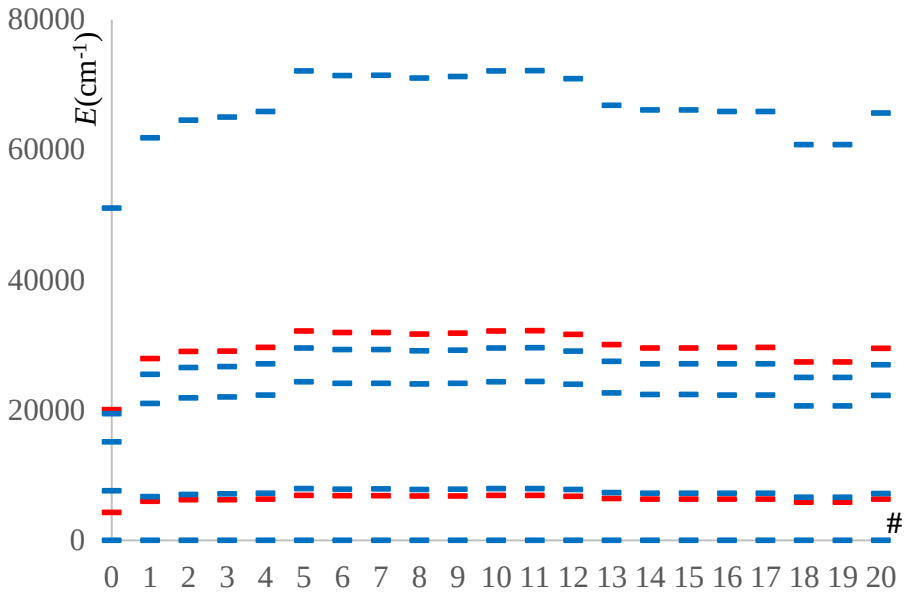

Figure S1. The spectral terms of the f^2 configuration of Pr(III) ion, relative to the ^{3}H ground state, computed with different basis sets. The labels on the abscissa correspond to the basis set given in the corresponding entry (order number) from in Table 4 in the main text. The levels marked on vertical axis correspond to the experimental data. The triplet states are drawn in blue, the singlets being in red lines.

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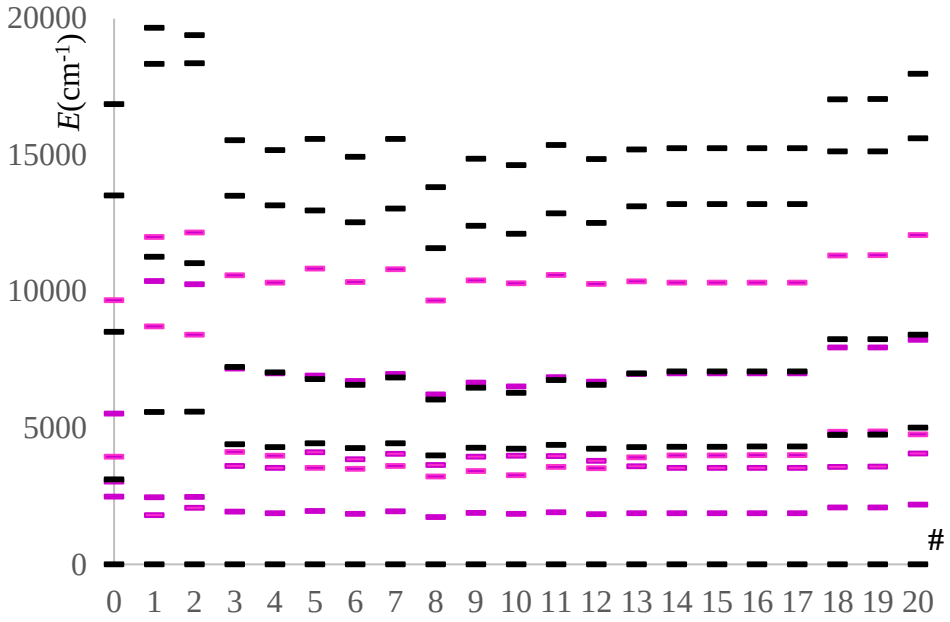

Figure S2. The spectral terms of the *fd* configuration of Pr(III) ion, relative to the ^{1}G lowest excited level. The singlets are drawn in black, while the triplets in magenta. The relative experimental values are marked on the vertical axis, the abscissa running on the order number of basis sets outlined in Table 4 from main text.