Electronic Supplementary Information for: The resolution of the weak-exchange limit made rigorous, simple and general in binuclear complexes

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S1 Supporting tables

Table S1 Matrix U used to translate $\hat{H}^{\mathrm{eff}}$ and $\hat{H}^{\mathrm{MS}}$ between the coupled-spin and uncoupled-spin bases.

U	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3/2,3/2\|$	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\langle 3/2,1/2\|$	0	$\frac{\sqrt{2}}{2}$	0	0	0	0	0	$\frac{\sqrt{2}}{2}$	0	0	0	0	0	0	0	0
$\langle 1/2,3/2\|$	0	$\frac{\sqrt{2}}{2}$	0	0	0	0	0	$-\frac{\sqrt{2}}{2}$	0	0	0	0	0	0	0	0
$\langle 3/2,-1/2\|$	0	0	$\frac{\sqrt{5}}{5}$	0	0	0	0	0	$\frac{\sqrt{2}}{2}$	0	0	0	$\frac{\sqrt{30}}{10}$	0	0	0
$\langle 1/2,1/2\|$	0	0	$\frac{\sqrt{15}}{5}$	0	0	0	0	0	0	0	0	0	$-\frac{\sqrt{10}}{5}$	0	0	0
$\langle -1/2,3/2\|$	0	0	$\frac{\sqrt{5}}{5}$	0	0	0	0	0	$-\frac{\sqrt{2}}{2}$	0	0	0	$\frac{\sqrt{30}}{10}$	0	0	0
$\langle 3/2,-3/2\|$	0	0	0	$\frac{\sqrt{5}}{10}$	0	0	0	0	0	$\frac{1}{2}$	0	0	0	$\frac{3\sqrt{5}}{10}$	0	$\frac{1}{2}$
$\langle 1/2,-1/2\|$	0	0	0	$\frac{3\sqrt{5}}{10}$	0	0	0	0	0	$\frac{1}{2}$	0	0	0	$-\frac{\sqrt{5}}{10}$	0	$-\frac{1}{2}$
$\langle -1/2,1/2\|$	0	0	0	$\frac{3\sqrt{5}}{10}$	0	0	0	0	0	$-\frac{1}{2}$	0	0	0	$-\frac{\sqrt{5}}{10}$	0	$\frac{1}{2}$
$\langle -3/2,3/2\|$	0	0	0	$\frac{\sqrt{5}}{10}$	0	0	0	0	0	$-\frac{1}{2}$	0	0	0	$\frac{3\sqrt{5}}{10}$	0	$-\frac{1}{2}$
$\langle 1/2,-3/2\|$	0	0	0	0	$\frac{\sqrt{5}}{5}$	0	0	0	0	0	$\frac{\sqrt{2}}{2}$	0	0	0	$\frac{\sqrt{30}}{10}$	0
$\langle -1/2,-1/2\|$	0	0	0	0	$\frac{\sqrt{15}}{5}$	0	0	0	0	0	0	0	0	0	$-\frac{\sqrt{10}}{5}$	0
$\langle -3/2,1/2\|$	0	0	0	0	$\frac{\sqrt{5}}{5}$	0	0	0	0	0	$-\frac{\sqrt{2}}{2}$	0	0	0	$\frac{\sqrt{30}}{10}$	0
$\langle -1/2,-3/2\|$	0	0	0	0	0	$\frac{\sqrt{2}}{2}$	0	0	0	0	0	$\frac{\sqrt{2}}{2}$	0	0	0	0
$\langle -3/2,-1/2\|$	0	0	0	0	0	$\frac{\sqrt{2}}{2}$	0	0	0	0	0	$-\frac{\sqrt{2}}{2}$	0	0	0	0
$\langle -3/2,-3/2\|$	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0

Table S2 SOCI energies, in cm^{-1}, corresponding to the 16 low-lying spin-orbit states of complex 1, calculated with various approaches.

SOCI state	SO-CASSCF	SO-NEVPT2	model//SO-NEVPT2	SO-DDCI2	model//SO-DDCI2
ψ_1	0.0	0.0	0.0	0.0	0.0
ψ_2	4.8	6.6	5.9	11.2	10.3
ψ_3	21.8	24.1	23.4	30.1	29.5
ψ_4	29.0	39.9	39.0	56.1	55.4
ψ_5	56.2	55.9	54.6	76.7	74.7
ψ_6	56.8	56.3	55.4	77.2	75.8
ψ_7	56.9	56.8	55.6	77.7	75.8
ψ_8	57.4	57.0	55.8	77.9	76.1
ψ_9	57.6	63.7	63.0	94.2	92.8
ψ_{10}	70.6	72.2	71.7	106.9	106.1
ψ_{11}	71.4	78.2	78.0	108.5	107.6
ψ_{12}	78.5	79.6	78.9	122.9	122.6
ψ_{13}	92.7	87.1	86.6	133.8	133.2
ψ_{14}	100.0	96.1	95.7	139.4	138.9
ψ_{15}	123.2	123.2	122.5	170.2	169.3
ψ_{16}	123.4	123.3	122.7	170.4	169.5

Table S3 Contribution of the $|S,M_S\rangle$ components of the low-lying $S = 0$, 1, 2, 3 states to the wavefunctions of the 16 low-energy spin-orbit states, obtained from a SO-NEVPT2 calculation on complex 1 in the arbitrary *xyz* frame.[a]

SOCI state	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
ψ_1	0	0	0	0	0	0	0	0.13	0	0	0	0.13	0	0	0	0.65
ψ_2	0.03	0	0	0	0	0	0.03	0	0	0	0	0	0.42	0.00	0.42	0
ψ_3	0	0.05	0	0.03	0	0.05	0	0	0	0	0	0	0	0.78	0	0
ψ_4	0.13	0	0.11	0	0.11	0	0.13	0	0	0	0	0	0.21	0	0.21	0
ψ_5	0	0	0	0	0	0	0	0.45	0.01	0.01	0.01	0.45	0	0	0	0
ψ_6	0	0	0	0	0	0	0	0	0.46	0	0.46	0	0	0	0	0
ψ_7	0	0	0	0	0	0	0	0.02	0.02	0.87	0.02	0.02	0	0	0	0
ψ_8	0	0	0	0	0	0	0	0.01	0.45	0.014	0.45	0.01	0	0	0	0
ψ_9	0	0.19	0.01	0.39	0.01	0.19	0	0	0	0	0	0	0	0.13	0	0
ψ_{10}	0	0.01	0.27	0.01	0.27	0.01	0	0	0	0	0	0	0.18	0	0.18	0
ψ_{11}	0.36	0	0.07	0.01	0.07	0	0.36	0	0	0	0	0	0.03	0	0.03	0
ψ_{12}	0	0	0	0	0	0	0	0.32	0	0.02	0	0.32	0	0	0	0.28
ψ_{13}	0	0.45	0.01	0	0.01	0.45	0	0	0	0	0	0	0	0	0	0
ψ_{14}	0.32	0.01	0.06	0	0.06	0.01	0.32	0	0	0	0	0	0.08	0	0.08	0
ψ_{15}	0	0.2	0.03	0.45	0.03	0.2	0	0	0	0	0	0	0	0.01	0	0
ψ_{16}	0.06	0.02	0.36	0.04	0.36	0.02	0.06	0	0	0	0	0	0	0	0	0

[a]The corresponding state energies are printed in Table S2.

Table S4 Contribution of the $|S,M_S\rangle$ components of the low-lying $S = 0$, 1, 2, 3 states to the wavefunctions of the 16 low-lying spin-orbit states, obtained from a SO-NEVPT2 calculation on complex 2 in the molecular PAF.[a]

SOCI state	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
ψ_1	0	0	0	0	0	0	0	0.02	0	0.23	0	0.02	0	0	0	0.65
ψ_2	0	0	0.03	0	0.03	0	0	0	0	0	0	0	0.43	0	0.43	0
ψ_3	0	0	0.07	0	0.07	0	0	0	0	0	0	0	0.39	0	0.39	0
ψ_4	0	0	0	0.5	0	0	0	0	0	0	0	0	0	0.41	0	0
ψ_5	0	0	0	0	0	0	0	0	0.46	0	0.46	0	0	0	0	0
ψ_6	0	0	0	0	0	0	0	0.46	0	0	0	0.46	0	0	0	0
ψ_7	0	0	0	0	0	0	0	0.4	0	0.11	0	0.4	0	0	0	0
ψ_8	0	0	0	0	0	0	0	0	0.46	0	0.46	0	0	0	0	0
ψ_9	0.01	0	0.39	0	0.39	0	0.01	0	0	0	0	0	0.07	0	0.07	0
ψ_{10}	0	0.17	0	0.23	0	0.17	0	0	0	0	0	0	0	0.36	0	0
ψ_{11}	0.01	0	0.42	0	0.42	0	0.01	0	0	0	0	0	0.03	0	0.03	0
ψ_{12}	0	0	0	0	0	0	0	0.04	0	0.57	0	0.04	0	0	0	0.28
ψ_{13}	0	0.46	0	0	0	0.46	0	0	0	0	0	0	0	0	0	0
ψ_{14}	0	0.29	0	0.19	0	0.29	0	0	0	0	0	0	0	0.16	0	0
ψ_{15}	0.46	0	0	0	0	0	0.46	0	0	0	0	0	0	0	0	0
ψ_{16}	0.45	0	0.01	0	0.01	0	0.45	0	0	0	0	0	0	0	0	0

[a]The corresponding state energies are printed in Table S2.

Table S5 Matrix elements of $\hat{H}^{\mathrm{MS}} = J\hat{S}_a\hat{S}_b + \hat{S}_a\bar{\bar{D}}_a\hat{S}_a + \hat{S}_b\bar{\bar{D}}_b\hat{S}_b$ for dicobalt(II) complexes in an arbitrary axis frame expressed in the $|S,M_S\rangle$ coupled spin-basis spanned by the $S=0,1,2,3$ spin functions. Notations such as D_{xx}^{a+b} and $-D_{xx}^{a-b}$ should be read as $D_{xx}^{a}+D_{xx}^{b}$ and $-D_{xx}^{a}+D_{xx}^{b}$ respectively. This Table is continued by Table S6. The symmetric anisotropy exchange part, $\hat{S}_a\bar{\bar{D}}_{ab}\hat{S}_b$, is provided separately in Table S7.

$\hat{H}^{MS}$	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$
$\langle 3,3\|$	$\frac{9J}{4}+\frac{3D_{xx}^{a+b}}{4}+\frac{3D_{yy}^{a+b}}{4}+\frac{9D_{zz}^{a+b}}{4}$	$\frac{\sqrt{6}\left(D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{2}$	$\frac{\sqrt{15}\left(D_{xx}^{a+b}-D_{yy}^{a+b}-2iD_{xy}^{a+b}\right)}{10}$	0	0	0	0
$\langle 3,2\|$	$\frac{\sqrt{6}\left(D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{2}$	$\frac{9J}{4}+\frac{5D_{xx}^{a+b}}{4}+\frac{5D_{yy}^{a+b}}{4}+\frac{5D_{zz}^{a+b}}{4}$	$\frac{3\sqrt{10}\left(D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{10}$	$\frac{\sqrt{30}\left(D_{xx}^{a+b}-D_{yy}^{a+b}-2iD_{xy}^{a+b}\right)}{10}$	0	0	0
$\langle 3,1\|$	$\frac{\sqrt{15}\left(D_{xx}^{a+b}-D_{yy}^{a+b}+2iD_{xy}^{a+b}\right)}{10}$	$\frac{3\sqrt{10}\left(D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{10}$	$\frac{9J}{4}+\frac{31D_{xx}^{a+b}}{20}+\frac{31D_{yy}^{a+b}}{20}+\frac{13D_{zz}^{a+b}}{20}$	$\frac{\sqrt{3}\left(D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{5}$	$\frac{3D_{xx}^{a+b}}{5}-\frac{3D_{yy}^{a+b}}{5}-\frac{6iD_{xy}^{a+b}}{5}$	0	0
$\langle 3,0\|$	0	$\frac{\sqrt{30}\left(D_{xx}^{a+b}+2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{10}$	$\frac{\sqrt{3}\left(D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{5}$	$\frac{9J}{4}+\frac{33D_{xx}^{a+b}}{20}+\frac{33D_{yy}^{a+b}}{20}+\frac{9D_{zz}^{a+b}}{20}$	$\frac{\sqrt{3}\left(-D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{5}$	$\frac{\sqrt{30}\left(D_{xx}^{a+b}-2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{10}$	0
$\langle 3,-1\|$	0	0	$\frac{3D_{xx}^{a+b}}{5}+\frac{6iD_{xy}^{a+b}}{5}-\frac{3D_{yy}^{a+b}}{5}$	$\frac{\sqrt{3}\left(-D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{5}$	$\frac{9J}{4}+\frac{31D_{xx}^{a+b}}{20}+\frac{31D_{yy}^{a+b}}{20}+\frac{13D_{zz}^{a+b}}{20}$	$\frac{3\sqrt{10}\left(-D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{10}$	$\frac{\sqrt{15}\left(D_{xx}^{a+b}-2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{10}$
$\langle 3,-2\|$	0	0	0	$\frac{\sqrt{30}\left(D_{xx}^{a+b}+2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{10}$	$\frac{\sqrt{15}\left(D_{xx}^{a+b}+2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{10}$	$\frac{9J}{4}+\frac{5D_{xx}^{a+b}}{4}+\frac{5D_{yy}^{a+b}}{4}+\frac{5D_{zz}^{a+b}}{4}$	$\frac{\sqrt{6}\left(-D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{2}$
$\langle 3,-3\|$	0	0	0	0	0	$\frac{\sqrt{6}\left(-D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{2}$	$\frac{9J}{4}+\frac{3D_{xx}^{a+b}}{4}+\frac{3D_{yy}^{a+b}}{4}+\frac{9D_{zz}^{a+b}}{4}$
$\langle 2,2\|$	$\frac{\sqrt{6}\left(-D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{2}$	$-\frac{D_{xx}^{a-b}}{2}-\frac{D_{yy}^{a-b}}{2}+D_{zz}^{a-b}$	$\frac{3\sqrt{10}\left(D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{10}$	$\frac{\sqrt{30}\left(D_{xx}^{a-b}-2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{20}$	0	0	0
$\langle 2,1\|$	$\frac{\sqrt{6}\left(-D_{xx}^{a-b}-2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{4}$	0	$\frac{\sqrt{10}\left(-D_{xx}^{a-b}-D_{yy}^{a-b}+2D_{zz}^{a-b}\right)}{10}$	$\frac{\sqrt{30}\left(D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{5}$	$\frac{3\sqrt{10}\left(D_{xx}^{a-b}-2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{20}$	0	0
$\langle 2,0\|$	0	$\frac{\sqrt{6}\left(-D_{xx}^{a-b}-2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{4}$	$\frac{\sqrt{15}\left(D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{5}$	0	$\frac{\sqrt{15}\left(D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{5}$	$\frac{\sqrt{6}\left(D_{xx}^{a-b}-2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{4}$	0
$\langle 2,-1\|$	0	0	$\frac{3\sqrt{10}\left(-D_{xx}^{a-b}-2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{20}$	$\frac{\sqrt{30}\left(D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{5}$	$\frac{\sqrt{10}\left(D_{xx}^{a-b}+D_{yy}^{a-b}-2D_{zz}^{a-b}\right)}{10}$	0	$\frac{\sqrt{6}\left(D_{xx}^{a-b}-2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{4}$
$\langle 2,-2\|$	0	0	0	$\frac{\sqrt{30}\left(-D_{xx}^{a-b}-2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{20}$	$\frac{3\sqrt{10}\left(D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{10}$	$\frac{D_{xx}^{a-b}}{2}+\frac{D_{yy}^{a-b}}{2}-D_{zz}^{a-b}$	$\frac{\sqrt{6}\left(D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{2}$
$\langle 1,1\|$	$\frac{3\sqrt{10}\left(D_{xx}^{a+b}+2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$	$\frac{\sqrt{15}\left(-D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{5}$	$\frac{\sqrt{6}\left(-D_{xx}^{a+b}-D_{yy}^{a+b}+2D_{zz}^{a+b}\right)}{10}$	$-\frac{3D_{xx}^{a+b}}{10}-\frac{3D_{yy}^{a+b}}{10}+\frac{3D_{zz}^{a+b}}{5}$	$\frac{\sqrt{6}\left(D_{xx}^{a+b}-2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$	0	0
$\langle 1,0\|$	0	$\frac{\sqrt{30}\left(D_{xx}^{a+b}+2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$	$\frac{2\sqrt{3}\left(-D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{5}$	$\frac{3\sqrt{2}\left(D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{10}$	$\frac{2\sqrt{3}\left(D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{5}$	$\frac{\sqrt{30}\left(D_{xx}^{a+b}-2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$	0
$\langle 1,-1\|$	0	0	$\frac{\sqrt{6}\left(D_{xx}^{a+b}+2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$	$\frac{3\sqrt{2}\left(-D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{10}$	$\frac{\sqrt{6}\left(-D_{xx}^{a+b}-D_{yy}^{a+b}+2D_{zz}^{a+b}\right)}{10}$	$\frac{\sqrt{15}\left(D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{5}$	$\frac{3\sqrt{10}\left(D_{xx}^{a+b}-2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$
$\langle 0,0\|$	0	0	0	0	0	0	0

	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$
$\langle 3,3\|$	$\frac{\sqrt{6}\left(-D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{2}$	$\frac{\sqrt{6}\left(-D_{xx}^{a-b}+2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{4}$	0	0	0
$\langle 3,2\|$	$-\frac{D_{xx}^{a-b}}{2}-\frac{D_{yy}^{a-b}}{2}+D_{zz}^{a-b}$	0	$\frac{\sqrt{6}\left(-D_{xx}^{a-b}+2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{4}$	0	0
$\langle 3,1\|$	$\frac{3\sqrt{10}\left(D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{10}$	$\frac{\sqrt{10}\left(-D_{xx}^{a-b}-D_{yy}^{a-b}+2D_{zz}^{a-b}\right)}{10}$	$\frac{\sqrt{15}\left(D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{5}$	$\frac{3\sqrt{10}\left(-D_{xx}^{a-b}+2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{20}$	0
$\langle 3,0\|$	$\frac{\sqrt{30}\left(D_{xx}^{a-b}+2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{20}$	$\frac{\sqrt{30}\left(D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{5}$	0	$\frac{\sqrt{30}\left(D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{5}$	$\frac{\sqrt{30}\left(-D_{xx}^{a-b}+2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{20}$
$\langle 3,-1\|$	0	$\frac{3\sqrt{10}\left(D_{xx}^{a-b}+2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{20}$	$\frac{\sqrt{15}\left(D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{5}$	$\frac{\sqrt{10}\left(D_{xx}^{a-b}+D_{yy}^{a-b}-2D_{zz}^{a-b}\right)}{10}$	$\frac{3\sqrt{10}\left(D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{10}$
$\langle 3,-2\|$	0	0	$\frac{\sqrt{6}\left(D_{xx}^{a-b}+2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{4}$	0	$\frac{D_{xx}^{a-b}}{2}+\frac{D_{yy}^{a-b}}{2}-D_{zz}^{a-b}$
$\langle 3,-3\|$	0	0	0	$\frac{\sqrt{6}\left(D_{xx}^{a-b}+2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{4}$	$\frac{\sqrt{6}\left(-D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{2}$
$\langle 2,2\|$	$-\frac{3J}{4}+\frac{5D_{xx}^{a+b}}{4}+\frac{5D_{yy}^{a+b}}{4}+\frac{5D_{zz}^{a+b}}{4}$	0	0	0	0
$\langle 2,1\|$	0	$-\frac{3J}{4}+\frac{5D_{xx}^{a+b}}{4}+\frac{5D_{yy}^{a+b}}{4}+\frac{5D_{zz}^{a+b}}{4}$	0	0	0
$\langle 2,0\|$	0	0	$-\frac{3J}{4}+\frac{5D_{xx}^{a+b}}{4}+\frac{5D_{yy}^{a+b}}{4}+\frac{5D_{zz}^{a+b}}{4}$	0	0
$\langle 2,-1\|$	0	0	0	$-\frac{3J}{4}+\frac{5D_{xx}^{a+b}}{4}+\frac{5D_{yy}^{a+b}}{4}+\frac{5D_{zz}^{a+b}}{4}$	0
$\langle 2,-2\|$	0	0	0	0	$-\frac{3J}{4}+\frac{5D_{xx}^{a+b}}{4}+\frac{5D_{yy}^{a+b}}{4}+\frac{5D_{zz}^{a+b}}{4}$
$\langle 1,1\|$	$\frac{\sqrt{15}\left(-D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{5}$	$\frac{\sqrt{15}\left(-D_{xx}^{a-b}-D_{yy}^{a-b}+2D_{zz}^{a-b}\right)}{10}$	$\frac{3\sqrt{10}\left(D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{10}$	$\frac{\sqrt{15}\left(D_{xx}^{a-b}-2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{10}$	0
$\langle 1,0\|$	$\frac{\sqrt{30}\left(-D_{xx}^{a-b}-2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{10}$	$\frac{\sqrt{30}\left(D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{10}$	0	$\frac{\sqrt{30}\left(D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{10}$	$\frac{\sqrt{30}\left(D_{xx}^{a-b}-2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{10}$
$\langle 1,-1\|$	0	$\frac{\sqrt{15}\left(-D_{xx}^{a-b}-2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{10}$	$\frac{3\sqrt{10}\left(D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{10}$	$\frac{\sqrt{15}\left(D_{xx}^{a-b}+D_{yy}^{a-b}-2D_{zz}^{a-b}\right)}{10}$	$\frac{\sqrt{15}\left(-D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{5}$
$\langle 0,0\|$	$\frac{\sqrt{6}\left(D_{xx}^{a+b}+2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{4}$	$\frac{\sqrt{6}\left(-D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{2}$	$-\frac{D_{xx}^{a+b}}{2}-\frac{D_{yy}^{a+b}}{2}+D_{zz}^{a+b}$	$\frac{\sqrt{6}\left(D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{2}$	$\frac{\sqrt{6}\left(D_{xx}^{a+b}-2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{4}$

Table S6 Table S5 continued.

H^{MS}	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3,3\|$	$\frac{3\sqrt{10}\left(D_{xx}^{a+b}-2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$	0	0	0
$\langle 3,2\|$	$\frac{\sqrt{15}\left(-D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{5}$	$\frac{\sqrt{30}\left(D_{xx}^{a+b}-2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$	0	0
$\langle 3,1\|$	$\frac{\sqrt{6}\left(-D_{xx}^{a+b}-D_{yy}^{a+b}+2D_{zz}^{a+b}\right)}{10}$	$\frac{2\sqrt{3}\left(-D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{5}$	$\frac{\sqrt{6}\left(D_{xx}^{a+b}-2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$	0
$\langle 3,0\|$	$\frac{3\sqrt{2}\left(D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{10}$	$-\frac{3D_{xx}^{a+b}}{10}-\frac{3D_{yy}^{a+b}}{10}+\frac{3D_{zz}^{a+b}}{5}$	$\frac{3\sqrt{2}\left(-D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{10}$	0
$\langle 3,-1\|$	$\frac{\sqrt{6}\left(D_{xx}^{a+b}+2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$	$\frac{2\sqrt{3}\left(D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{5}$	$\frac{\sqrt{6}\left(-D_{xx}^{a+b}-D_{yy}^{a+b}+2D_{zz}^{a+b}\right)}{10}$	0
$\langle 3,-2\|$	0	$\frac{\sqrt{30}\left(D_{xx}^{a+b}+2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$	$\frac{\sqrt{15}\left(D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{5}$	0
$\langle 3,-3\|$	0	0	$\frac{3\sqrt{10}\left(D_{xx}^{a+b}+2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{20}$	0
$\langle 2,2\|$	$\frac{\sqrt{15}\left(-D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{5}$	$\frac{\sqrt{30}\left(-D_{xx}^{a-b}+2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{10}$	0	$\frac{\sqrt{6}\left(D_{xx}^{a+b}-2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{4}$
$\langle 2,1\|$	$\frac{\sqrt{15}\left(-D_{xx}^{a-b}-D_{yy}^{a-b}+2D_{zz}^{a-b}\right)}{10}$	$\frac{\sqrt{30}\left(D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{10}$	$\frac{\sqrt{15}\left(-D_{xx}^{a-b}+2iD_{xy}^{a-b}+D_{yy}^{a-b}\right)}{10}$	$\frac{\sqrt{6}\left(-D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{2}$
$\langle 2,0\|$	$\frac{3\sqrt{10}\left(D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{10}$	0	$\frac{3\sqrt{10}\left(D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{10}$	$-\frac{D_{xx}^{a+b}}{2}-\frac{D_{yy}^{a+b}}{2}+D_{zz}^{a+b}$
$\langle 2,-1\|$	$\frac{\sqrt{15}\left(D_{xx}^{a-b}+2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{10}$	$\frac{\sqrt{30}\left(D_{xz}^{a-b}+iD_{yz}^{a-b}\right)}{10}$	$\frac{\sqrt{15}\left(D_{xx}^{a-b}+D_{yy}^{a-b}-2D_{zz}^{a-b}\right)}{10}$	$\frac{\sqrt{6}\left(D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{2}$
$\langle 2,-2\|$	0	$\frac{\sqrt{30}\left(D_{xx}^{a-b}+2iD_{xy}^{a-b}-D_{yy}^{a-b}\right)}{10}$	$\frac{\sqrt{15}\left(-D_{xz}^{a-b}-iD_{yz}^{a-b}\right)}{5}$	$\frac{\sqrt{6}\left(D_{xx}^{a+b}+2iD_{xy}^{a+b}-D_{yy}^{a+b}\right)}{4}$
$\langle 1,1\|$	$-\frac{11J}{4}+\frac{29D_{xx}^{a+b}}{20}+\frac{29D_{yy}^{a+b}}{20}+\frac{17D_{zz}^{a+b}}{20}$	$\frac{3\sqrt{2}\left(-D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{5}$	$-\frac{3D_{xx}^{a+b}}{5}+\frac{6iD_{xy}^{a+b}}{5}+\frac{3D_{yy}^{a+b}}{5}$	0
$\langle 1,0\|$	$\frac{3\sqrt{2}\left(-D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{5}$	$-\frac{11J}{4}+\frac{17D_{xx}^{a+b}}{20}+\frac{17D_{yy}^{a+b}}{20}+\frac{41D_{zz}^{a+b}}{20}$	$\frac{3\sqrt{2}\left(D_{xz}^{a+b}-iD_{yz}^{a+b}\right)}{5}$	0
$\langle 1,-1\|$	$-\frac{3D_{xx}^{a+b}}{5}-\frac{6iD_{xy}^{a+b}}{5}+\frac{3D_{yy}^{a+b}}{5}$	$\frac{3\sqrt{2}\left(D_{xz}^{a+b}+iD_{yz}^{a+b}\right)}{5}$	$-\frac{11J}{4}+\frac{29D_{xx}^{a+b}}{20}+\frac{29D_{yy}^{a+b}}{20}+\frac{17D_{zz}^{a+b}}{20}$	0
$\langle 0,0\|$	0	0	0	$-\frac{15J}{4}+\frac{5D_{xx}^{a+b}}{4}+\frac{5D_{yy}^{a+b}}{4}+\frac{5D_{zz}^{a+b}}{4}$

Table S7 Matrix elements of $\hat{H}^{\mathrm{MS}}$ for dicobalt(II) complexes in an arbitrary axis frame expressed in the $|S,M_S\rangle$ coupled spin-basis defined by $S=0,1,2,3$ spin functions. This table provides the symmetric anisotropy exchange part, $\hat{S}_a\bar{\bar{D}}_{ab}\hat{S}_b$.

H^{MS}	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$
$\langle 3,3\|$	$\frac{9D_{zz}^{ab}}{4}$	$\frac{3\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	$\frac{3\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	0	$\frac{3D_{xx}^{ab}}{4}-\frac{3iD_{xy}^{ab}}{2}-\frac{3D_{yy}^{ab}}{4}$	0	0
$\langle 3,2\|$	$\frac{3\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	$\frac{3D_{zz}^{ab}}{4}$	$\frac{3D_{xx}^{ab}}{4}+\frac{3D_{yy}^{ab}}{4}$	$\frac{3D_{xz}^{ab}}{2}-\frac{3iD_{yz}^{ab}}{2}$	$\frac{\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	0	0
$\langle 3,1\|$	$\frac{3\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	$\frac{3D_{xx}^{ab}}{4}+\frac{3D_{yy}^{ab}}{4}$	$\frac{3D_{zz}^{ab}}{4}$	0	$\frac{\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	$\frac{3D_{xz}^{ab}}{2}-\frac{3iD_{yz}^{ab}}{2}$	0
$\langle 3,0\|$	0	$\frac{3D_{xz}^{ab}}{2}+\frac{3iD_{yz}^{ab}}{2}$	0	$-\frac{3D_{zz}^{ab}}{4}$	$\frac{\sqrt{3}\left(D_{xx}^{ab}+D_{yy}^{ab}\right)}{2}$	0	$\frac{3\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$
$\langle 3,-1\|$	$\frac{3D_{xx}^{ab}}{4}+\frac{3iD_{xy}^{ab}}{2}-\frac{3D_{yy}^{ab}}{4}$	$\frac{\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	$\frac{\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	$\frac{\sqrt{3}\left(D_{xx}^{ab}+D_{yy}^{ab}\right)}{2}$	$\frac{D_{zz}^{ab}}{4}$	$\frac{\sqrt{3}\left(D_{xx}^{ab}+D_{yy}^{ab}\right)}{2}$	0
$\langle 3,-2\|$	0	0	$\frac{3D_{xz}^{ab}}{2}+\frac{3iD_{yz}^{ab}}{2}$	0	$\frac{\sqrt{3}\left(D_{xx}^{ab}+D_{yy}^{ab}\right)}{2}$	$-\frac{3D_{zz}^{ab}}{4}$	0
$\langle 3,-3\|$	0	0	0	$\frac{3\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	0	0	$-\frac{9D_{zz}^{ab}}{4}$
$\langle 2,2\|$	0	$\frac{\sqrt{3}\left(D_{xx}^{ab}+2iD_{xy}^{ab}-D_{yy}^{ab}\right)}{2}$	0	$-\frac{\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	$\frac{D_{xz}^{ab}}{2}+\frac{iD_{yz}^{ab}}{2}$	0	$\frac{3D_{xx}^{ab}}{4}+\frac{3D_{yy}^{ab}}{4}$
$\langle 2,1\|$	0	0	$\frac{\sqrt{3}\left(D_{xx}^{ab}+2iD_{xy}^{ab}-D_{yy}^{ab}\right)}{2}$	0	$\frac{D_{xz}^{ab}}{2}+\frac{iD_{yz}^{ab}}{2}$	$-\frac{3\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	0
$\langle 2,0\|$	0	0	0	0	0	$\frac{3\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	0
$\langle 2,-1\|$	0	0	0	$\frac{3D_{xx}^{ab}}{4}+\frac{3iD_{xy}^{ab}}{2}-\frac{3D_{yy}^{ab}}{4}$	0	0	$-\frac{3\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$
$\langle 2,-2\|$	0	0	0	0	$D_{xx}^{ab}+2iD_{xy}^{ab}-D_{yy}^{ab}$	0	0
$\langle 1,1\|$	0	0	0	0	0	$\frac{3D_{xx}^{ab}}{4}+\frac{3iD_{xy}^{ab}}{2}-\frac{3D_{yy}^{ab}}{4}$	
$\langle 1,0\|$	0	0	0	0	0	0	0
$\langle 1,-1\|$	0	0	0	0	0	0	0
$\langle 0,0\|$	0	0	0	0	0	0	0

	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3,3\|$	0	0	0	0	0	0	0	0	0
$\langle 3,2\|$	$\frac{\sqrt{3}\left(D_{xx}^{ab}-2iD_{xy}^{ab}-D_{yy}^{ab}\right)}{2}$	0	0	0	0	0	0	0	0
$\langle 3,1\|$	0	$\frac{\sqrt{3}\left(D_{xx}^{ab}-2iD_{xy}^{ab}-D_{yy}^{ab}\right)}{2}$	0	0	0	0	0	0	0
$\langle 3,0\|$	$-\frac{\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	0	0	$\frac{3D_{xx}^{ab}}{4}-\frac{3iD_{xy}^{ab}}{2}-\frac{3D_{yy}^{ab}}{4}$	0	0	0	0	0
$\langle 3,-1\|$	$\frac{D_{xz}^{ab}}{2}-\frac{iD_{yz}^{ab}}{2}$	$\frac{D_{xz}^{ab}}{2}-\frac{iD_{yz}^{ab}}{2}$	0	0	$D_{xx}^{ab}-2iD_{xy}^{ab}-D_{yy}^{ab}$	0	0	0	0
$\langle 3,-2\|$	0	$-\frac{3\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	$\frac{3\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	0	0	$\frac{3D_{xx}^{ab}}{4}-\frac{3iD_{xy}^{ab}}{2}-\frac{3D_{yy}^{ab}}{4}$	0	0	0
$\langle 3,-3\|$	$\frac{3D_{xx}^{ab}}{4}+\frac{3D_{yy}^{ab}}{4}$	0	0	$-\frac{3\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	0	0	0	0	0
$\langle 2,2\|$	$-\frac{D_{zz}^{ab}}{4}$	$D_{xx}^{ab}-D_{yy}^{ab}$	0	$\frac{\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	$-\frac{D_{xz}^{ab}}{2}+\frac{iD_{yz}^{ab}}{2}$	0	$\frac{\sqrt{3}\left(D_{xx}^{ab}-2iD_{xy}^{ab}-D_{yy}^{ab}\right)}{2}$	0	0
$\langle 2,1\|$	$D_{xx}^{ab}-D_{yy}^{ab}$	$-\frac{D_{zz}^{ab}}{4}$	$\frac{3D_{xx}^{ab}}{4}+\frac{3D_{yy}^{ab}}{4}$	0	$-\frac{D_{xz}^{ab}}{2}+\frac{iD_{yz}^{ab}}{2}$	$\frac{\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	0	$\frac{\sqrt{3}\left(D_{xx}^{ab}-2iD_{xy}^{ab}-D_{yy}^{ab}\right)}{2}$	0
$\langle 2,0\|$	0	$\frac{3D_{xx}^{ab}}{4}+\frac{3D_{yy}^{ab}}{4}$	$-\frac{9D_{zz}^{ab}}{4}$	0	0	$-\frac{3\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	0	0	0
$\langle 2,-1\|$	$\frac{\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	0	0	$-\frac{3D_{zz}^{ab}}{4}$	$\frac{\sqrt{3}\left(D_{xx}^{ab}+D_{yy}^{ab}\right)}{2}$	0	$-\frac{3D_{xz}^{ab}}{2}+\frac{3iD_{yz}^{ab}}{2}$	0	0
$\langle 2,-2\|$	$-\frac{D_{xz}^{ab}}{2}-\frac{iD_{yz}^{ab}}{2}$	$-\frac{D_{xz}^{ab}}{2}-\frac{iD_{yz}^{ab}}{2}$	0	$\frac{\sqrt{3}\left(D_{xx}^{ab}+D_{yy}^{ab}\right)}{2}$	$\frac{D_{zz}^{ab}}{4}$	$\frac{\sqrt{3}\left(D_{xx}^{ab}+D_{yy}^{ab}\right)}{2}$	$-\frac{\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	$-\frac{\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	$\frac{3D_{xx}^{ab}}{4}-\frac{3iD_{xy}^{ab}}{2}-\frac{3D_{yy}^{ab}}{4}$
$\langle 1,1\|$	0	$\frac{\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	$-\frac{3\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	0	$\frac{\sqrt{3}\left(D_{xx}^{ab}+D_{yy}^{ab}\right)}{2}$	$-\frac{3D_{zz}^{ab}}{4}$	0	$-\frac{3D_{xz}^{ab}}{2}+\frac{3iD_{yz}^{ab}}{2}$	0
$\langle 1,0\|$	$\frac{\sqrt{3}\left(D_{xx}^{ab}+2iD_{xy}^{ab}-D_{yy}^{ab}\right)}{2}$	0	0	$-\frac{3D_{xz}^{ab}}{2}-\frac{3iD_{yz}^{ab}}{2}$	$-\frac{\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	0	$\frac{3D_{zz}^{ab}}{4}$	$\frac{3D_{xx}^{ab}}{4}+\frac{3D_{yy}^{ab}}{4}$	$-\frac{3\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$
$\langle 1,-1\|$	0	$\frac{\sqrt{3}\left(D_{xx}^{ab}+2iD_{xy}^{ab}-D_{yy}^{ab}\right)}{2}$	0	0	$-\frac{3D_{xz}^{ab}}{2}-\frac{3iD_{yz}^{ab}}{2}$	$\frac{3D_{xx}^{ab}}{4}+\frac{3D_{yy}^{ab}}{4}$	$\frac{3D_{zz}^{ab}}{4}$	$-\frac{3\sqrt{3}\left(D_{xz}^{ab}-iD_{yz}^{ab}\right)}{4}$	
$\langle 0,0\|$	0	0	0	0	$\frac{3D_{xx}^{ab}}{4}+\frac{3iD_{xy}^{ab}}{2}-\frac{3D_{yy}^{ab}}{4}$	0	$-\frac{3\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	$-\frac{3\sqrt{3}\left(D_{xz}^{ab}+iD_{yz}^{ab}\right)}{4}$	$\frac{9D_{zz}^{ab}}{4}$

Table S8 Complex 1: Matrix elements, in cm^{-1}, of $\hat{H}^{\text{eff}}$ expressed in the $|S,M_S\rangle$ coupled-spin basis, obtained from a SO-NEVPT2 calculation on complex 1 in the molecular PAF.

$\hat{H}^{\text{MS}}$	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3,3\|$	58.2	0	5.1	0	0	0	0	0	0	0	0	0	$-7.8+0.6i$	0	0	0
$\langle 3,2\|$	0	23.3	0	7.2	0	0	0	0	0	0	0	0	0	$-4.5+0.3i$	0	0
$\langle 3,1\|$	5.1	0	2.5	0	7.9	0	0	0	0	0	0	0	-16.7	0	$-2.0+0.1i$	0
$\langle 3,0\|$	0	7.2	0	-4.5	0	7.2	0	0	0	0	0	0	0	-20.4	0	0
$\langle 3,-1\|$	0	0	7.9	0	2.5	0	5.1	0	0	0	0	0	$-2.0-0.1i$	0	-16.7	0
$\langle 3,-2\|$	0	0	0	7.2	0	23.3	0	0	0	0	0	0	0	$-4.5-0.3i$	0	0
$\langle 3,-3\|$	0	0	0	0	5.1	0	58.2	0	0	0	0	0	0	0	$-7.8-0.6i$	0
$\langle 2,2\|$	0	0	0	0	0	0	0	-7.4	$0.1i$	$-0.4+0.2i$	0	0	0	0	0	$-9.6+0.5i$
$\langle 2,1\|$	0	0	0	0	0	0	0	$-0.1i$	-7.3	0	$-0.5+0.3i$	0	0	0	0	$-0.1+0.1i$
$\langle 2,0\|$	0	0	0	0	0	0	0	$-0.4-0.2i$	0	-7.3	0	$-0.4+0.2i$	0	0	0	-33.7
$\langle 2,-1\|$	0	0	0	0	0	0	0	0	$-0.5-0.3i$	0	-7.3	$-0.1i$	0	0	0	$0.1+0.1i$
$\langle 2,-2\|$	0	0	0	0	0	0	0	0	0	$-0.4-0.2i$	$0.1i$	-7.4	0	0	0	$-9.6-0.5i$
$\langle 1,1\|$	$-7.8-0.6i$	0	-16.7	0	$-2.0+0.1i$	0	0	0	0	0	0	0	-42.4	0.1	$-9.3+0.4i$	0
$\langle 1,0\|$	0	$-4.5-0.3i$	0	-20.4	0	$-4.5+0.3i$	0	0	0	0	0	0	0.1	-1.8	-0.1	0
$\langle 1,-1\|$	0	0	$-2.0-0.1i$	0	-16.7	0	$-7.8+0.6i$	0	0	0	0	0	$-9.3-0.4i$	-0.1	-42.4	0
$\langle 0,0\|$	0	0	0	0	0	0	0	$-9.6-0.5i$	$-0.1-0.1i$	-33.7	$0.1-0.1i$	$-9.6+0.5i$	0	0	0	-40.2

Table S9 Complex 1: Matrix elements,in cm^{-1}, of $\hat{H}^{\text{eff}}$ (Table S8) expressed in the uncoupled-spin basis, $|M_{Sa},M_{Sb}\rangle$.

$\hat{H}^{\text{MS}}$	$\|\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{3}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},-\frac{3}{2}\rangle$
$\langle\frac{3}{2},\frac{3}{2}\|$	58.2	0	0	$-2.0+0.3i$	$8.8-0.3i$	$-2.0+0.3i$	0	0	0	0	0	0	0	0	0	0
$\langle\frac{3}{2},\frac{1}{2}\|$	0	8.0	15.4	0	0	0	$-4.5+0.4i$	$7.3-0.1i$	$0.9+0.1i$	$2.6-0.1i$	0	0	0	0	0	0
$\langle\frac{1}{2},\frac{3}{2}\|$	0	15.4	8.0	0	0	0	$2.6-0.1i$	$0.9+0.1i$	$7.3-0.1i$	$-4.5+0.4i$	0	0	0	0	0	0
$\langle\frac{3}{2},-\frac{1}{2}\|$	$-2.0-0.3i$	0	0	-24.0	13.2	-16.7	0	0	0	$-0.1i$	$-2.5+0.3i$	$5.7-0.1i$	$-1.9+0.1i$	0	0	0
$\langle\frac{1}{2},\frac{1}{2}\|$	$8.8+0.3i$	0	0	13.2	0.9	13.2	0	0	0	0	$5.7-0.1i$	$3.0+0.1i$	$5.7-0.1i$	0	0	0
$\langle-\frac{1}{2},\frac{3}{2}\|$	$-2.0-0.3i$	0	0	-16.7	13.2	-24.0	$-0.1i$	0	0	0	$-1.9+0.1i$	$5.7-0.1i$	$-2.5+0.3i$	0	0	0
$\langle\frac{3}{2},-\frac{3}{2}\|$	0	$-4.5-0.4i$	$2.6+0.1i$	0	0	$0.1i$	-35.9	-0.4	-16.8	21.6	0	0	$0.1i$	$-4.5+0.4i$	$2.6-0.1i$	0
$\langle\frac{1}{2},-\frac{1}{2}\|$	0	$7.3+0.1i$	$0.9-0.1i$	0	0	0	-0.4	9.0	-1.0	-16.8	0	0	0	$7.3-0.1i$	$0.9+0.1i$	0
$\langle-\frac{1}{2},\frac{1}{2}\|$	0	$0.9-0.1i$	$7.3+0.1i$	0	0	0	-16.8	-1.0	9.0	-0.4	0	0	0	$0.9+0.1i$	$7.3-0.1i$	0
$\langle-\frac{3}{2},\frac{3}{2}\|$	0	$2.6+0.1i$	$-4.5-0.4i$	$0.1i$	0	0	21.6	-16.8	-0.4	-35.9	$0.1i$	0	0	$2.6-0.1i$	$-4.5+0.4i$	0
$\langle\frac{1}{2},-\frac{3}{2}\|$	0	0	0	$-2.5-0.3i$	$5.7+0.1i$	$-1.9-0.1i$	0	0	0	$-0.1i$	-24.0	13.2	-16.7	0	0	$-2.0+0.3i$
$\langle-\frac{1}{2},-\frac{1}{2}\|$	0	0	0	$5.7+0.1i$	$3.0-0.1i$	$5.7+0.1i$	0	0	0	0	13.2	0.9	13.2	0	0	$8.8-0.3i$
$\langle-\frac{3}{2},\frac{1}{2}\|$	0	0	0	$-1.9-0.1i$	$5.7+0.1i$	$-2.5-0.3i$	$-0.1i$	0	0	0	-16.7	13.2	-24.0	0	0	$-2.0+0.3i$
$\langle-\frac{1}{2},-\frac{3}{2}\|$	0	0	0	0	0	0	$-4.5-0.4i$	$7.3+0.1i$	$0.9-0.1i$	$2.6+0.1i$	0	0	0	8.0	15.4	0
$\langle-\frac{3}{2},-\frac{1}{2}\|$	0	0	0	0	0	0	$2.6+0.1i$	$0.9-0.1i$	$7.3+0.1i$	$-4.5-0.4i$	0	0	0	15.4	8.0	0
$\langle-\frac{3}{2},-\frac{3}{2}\|$	0	0	0	0	0	0	0	0	0	0	$-2.0-0.3i$	$8.8+0.3i$	$-2.0-0.3i$	0	0	58.2

Table S10 Complex 1: Matrix elements, in cm^{-1}, of $\hat{H}^{MS}=J\hat{S}_a\hat{S}_b+\hat{S}_a\bar{\bar{D}}_a\hat{S}_a+\hat{S}_b\bar{\bar{D}}_b\hat{S}_b$ expressed in the $|S,M_S\rangle$ coupled-spin basis, obtained with the spin-free NEVPT2 $J=11.2$ cm^{-1} and the SO-NEVPT2 ZFS parameters $D_a=D_b=17.4$ cm^{-1} and $E_a=E_b=3.7$ cm^{-1}.

$\hat{H}^{MS}$	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3,3\|$	59.8	−0.1	5.7	0	0	0	0	0	0	0	0	0	7.0	0	0	0
$\langle 3,2\|$	−0.1	25.1	−0.1	8.1	0	0	0	0	0	0	0	0	0.1	4.0	0	0
$\langle 3,1\|$	5.7	−0.1	4.3	0	8.9	0	0	0	0	0	0	0	17.0	0	1.8	0
$\langle 3,0\|$	0	8.1	0	−2.7	0	8.1	0	0	0	0	0	0	0	20.8	0	0
$\langle 3,-1\|$	0	0	8.9	0	4.3	0.1	5.7	0	0	0	0	0	1.8	0	17.0	0
$\langle 3,-2\|$	0	0	0	8.1	0.1	25.1	0.1	0	0	0	0	0	0	4.0	−0.1	0
$\langle 3,-3\|$	0	0	0	0	5.7	0.1	59.8	0	0	0	0	0	0	0	7.0	0
$\langle 2,2\|$	0	0	0	0	0	0	0	−8.4	0	0	0	0	0	0	0	9.1
$\langle 2,1\|$	0	0	0	0	0	0	0	0	−8.4	0	0	0	0	0	0	0.1
$\langle 2,0\|$	0	0	0	0	0	0	0	0	0	−8.4	0	0	0	0	0	34.7
$\langle 2,-1\|$	0	0	0	0	0	0	0	0	0	0	−8.4	0	0	0	0	−0.1
$\langle 2,-2\|$	0	0	0	0	0	0	0	0	0	0	0	−8.4	0	0	0	9.1
$\langle 1,1\|$	7.0	0.1	17.0	0	1.8	0	0	0	0	0	0	0	−44.6	0.1	−8.9	0
$\langle 1,0\|$	0	4.0	0	20.8	0	4.0	0	0	0	0	0	0	0.1	−2.9	−0.1	0
$\langle 1,-1\|$	0	0	1.8	0	17.0	−0.1	7.0	0	0	0	0	0	−8.9	−0.1	−44.6	0
$\langle 0,0\|$	0	0	0	0	0	0	0	9.1	0.1	34.7	−0.1	9.1	0	0	0	−41.9

Table S11 Complex 1: Numerical matrix elements (cm^{-1}) of $\hat{H}^{MS}=J\hat{S}_a\hat{S}_b+\hat{S}_a\bar{\bar{D}}_a\hat{S}_a+\hat{S}_b\bar{\bar{D}}_b\hat{S}_b$ expressed in the $|M_{Sa},M_{Sb}\rangle$ uncoupled-spin basis, obtained with the spin-free NEVPT2 $J=11.2$ cm^{-1} and the SO-NEVPT2 ZFS parameters $D_a=D_b=17.4$ cm^{-1} and $E_a=E_b=3.7$ cm^{-1}.

$\hat{H}^{MS}$	$\|\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{3}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},-\frac{3}{2}\rangle$
$\langle\frac{3}{2},\frac{3}{2}\|$	59.8	−0.1	−0.1	6.4	0	6.4	0	0	0	0	0	0	0	0	0	0
$\langle\frac{3}{2},\frac{1}{2}\|$	−0.1	8.4	16.7	0	−0.1	0	6.4	0	6.4	0	0	0	0	0	0	0
$\langle\frac{1}{2},\frac{3}{2}\|$	−0.1	16.7	8.4	0	−0.1	0	0	6.4	0	6.4	0	0	0	0	0	0
$\langle\frac{3}{2},-\frac{1}{2}\|$	6.4	0	0	−8.4	19.3	0	0.1	−0.1	0	0	0	6.4	0	0	0	0
$\langle\frac{1}{2},\frac{1}{2}\|$	0	−0.1	−0.1	19.3	−31.9	19.3	0	0	0	0	6.4	0	6.4	0	0	0
$\langle-\frac{1}{2},\frac{3}{2}\|$	6.4	0	0	0	19.3	−8.4	0	0	−0.1	0.1	0	6.4	0	0	0	0
$\langle\frac{3}{2},-\frac{3}{2}\|$	0	6.4	0	0.1	0	0	9.6	16.7	0	0	−0.1	0	0	6.4	0	0
$\langle\frac{1}{2},-\frac{1}{2}\|$	0	0	6.4	−0.1	0	0	16.7	−37.5	22.3	0	0.1	0	0	0	6.4	0
$\langle-\frac{1}{2},\frac{1}{2}\|$	0	6.4	0	0	0	−0.1	0	22.3	−37.5	16.7	0	0	0.1	6.4	0	0
$\langle-\frac{3}{2},\frac{3}{2}\|$	0	0	6.4	0	0	0.1	0	0	16.7	9.6	0	0	−0.1	0	6.4	0
$\langle\frac{1}{2},-\frac{3}{2}\|$	0	0	0	0	6.4	0	−0.1	0.1	0	0	−8.4	19.3	0	0	0	6.4
$\langle-\frac{1}{2},-\frac{1}{2}\|$	0	0	0	6.4	0	6.4	0	0	0	0	19.3	−31.9	19.3	0.1	0.1	0
$\langle-\frac{3}{2},\frac{1}{2}\|$	0	0	0	0	6.4	0	0	0	0.1	−0.1	0	19.3	−8.4	0	0	6.4
$\langle-\frac{1}{2},-\frac{3}{2}\|$	0	0	0	0	0	0	6.4	0	6.4	0	0	0.1	0	8.4	16.7	0.1
$\langle-\frac{3}{2},-\frac{1}{2}\|$	0	0	0	0	0	0	0	6.4	0	6.4	0	0.1	0	16.7	8.4	0.1
$\langle-\frac{3}{2},-\frac{3}{2}\|$	0	0	0	0	0	0	0	0	0	0	6.4	0	6.4	0.1	0.1	59.8

Table S12 Complex 1: Revised matrix elements. in cm^{-1}, of $\hat{H}^{\text{eff}}$ expressed in the $|S,M_S\rangle$ coupled-spin basis, obtained from a SO-NEVPT2 calculation on complex 1 in the molecular PAF. It was generated from the original $\hat{H}^{\text{eff}}$ matrix of Table S8 by multiplying by a factor of -1 the elements of the $\langle 0,0|\ \hat{H}^{\text{eff}}\,|2,M_S\rangle$ and $\langle 1,M_S|\ \hat{H}^{\text{eff}}\,|3,M_S\rangle$ blocks.

$\hat{H}^{\text{MS}}$	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3,3\|$	58.2	0	5.1	0	0	0	0	0	0	0	0	0	$7.8-0.6i$	0	0	0
$\langle 3,2\|$	0	23.3	0	7.2	0	0	0	0	0	0	0	0	0	$4.5-0.3i$	0	0
$\langle 3,1\|$	5.1	0	2.5	0	7.9	0	0	0	0	0	0	0	16.7	0	$2.0-0.1i$	0
$\langle 3,0\|$	0	7.2	0	−4.5	0	7.2	0	0	0	0	0	0	0	20.4	0	0
$\langle 3,-1\|$	0	0	7.9	0	2.5	0	5.1	0	0	0	0	0	$2.0+0.1i$	0	16.7	0
$\langle 3,-2\|$	0	0	0	7.2	0	23.3	0	0	0	0	0	0	0	$4.5+0.3i$	0	0
$\langle 3,-3\|$	0	0	0	0	5.1	0	58.2	0	0	0	0	0	0	0	$7.8+0.6i$	0
$\langle 2,2\|$	0	0	0	0	0	0	0	−7.4	$-0.1i$	$0.4-0.2i$	0	0	0	0	0	$9.6-0.5i$
$\langle 2,1\|$	0	0	0	0	0	0	0	$0.1i$	−7.3	0	$0.5-0.3i$	0	0	0	0	$0.1-0.1i$
$\langle 2,0\|$	0	0	0	0	0	0	0	$0.4+0.2i$	0	−7.3	0	$0.4-0.2i$	0	0	0	33.7
$\langle 2,-1\|$	0	0	0	0	0	0	0	0	$0.5+0.3i$	0	−7.3	$0.1i$	0	0	0	$-0.1-0.1i$
$\langle 2,-2\|$	0	0	0	0	0	0	0	0	0	$-0.4-0.2i$	$-0.1i$	−7.4	0	0	0	$9.6+0.5i$
$\langle 1,1\|$	$7.8+0.6i$	0	16.7	0	$2.0-0.1i$	0	0	0	0	0	0	0	−42.4	0.1	$-9.3+0.4i$	0
$\langle 1,0\|$	0	$4.5+0.3i$	0	20.4	0	$4.5-0.3i$	0	0	0	0	0	0	0.1	−1.8	−0.1	0
$\langle 1,-1\|$	0	0	$2.0+0.1i$	0	16.7	0	$7.8-0.6i$	0	0	0	0	0	$-9.3-0.4i$	−0.1	−42.4	0
$\langle 0,0\|$	0	0	0	0	0	0	0	$9.6+0.5i$	$0.1+0.1i$	33.7	$-0.1+0.1i$	$9.6-0.5i$	0	0	0	−40.2

Table S13 Complex 1: Matrix elements, in cm^{-1}, of $\hat{H}^{\text{eff}}$ expressed in the $|M_{Sa},M_{Sb}\rangle$ uncoupled-spin basis, obtained by basis transformation of the sign-revised, coupled-spin basis $\hat{H}^{\text{eff}}$ of Table S12.

$\hat{H}^{\text{MS}}$	$\|\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{3}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},-\frac{3}{2}\rangle$
$\langle\frac{3}{2},\frac{3}{2}\|$	58.2	0	0	$6.5-0.3i$	$-1.0+0.4i$	$6.5-0.3i$	0	0	0	0	0	0	0	0	0	0
$\langle\frac{3}{2},\frac{1}{2}\|$	0	8.0	15.4	0	0	0	$6.8-0.4i$	$-0.5+0.2i$	5.9	$-0.3+0.1i$	0	0	0	0	0	0
$\langle\frac{1}{2},\frac{3}{2}\|$	0	15.4	8.0	0	0	0	$-0.3+0.1i$	5.9	$-0.5+0.2i$	$6.8-0.4i$	0	0	0	0	0	0
$\langle\frac{3}{2},-\frac{1}{2}\|$	$6.5+0.3i$	0	0	−7.7	17.9	−0.4	0	0	0	0	$-0.1i$	$6.2-0.2i$	$-0.5+0.2i$	0	0	0
$\langle\frac{1}{2},\frac{1}{2}\|$	$-1.0-0.4i$	0	0	17.9	−31.8	17.9	0	0	0	0	$6.2-0.2i$	$-0.9+0.3i$	$6.2-0.2i$	0	0	0
$\langle-\frac{1}{2},\frac{3}{2}\|$	$6.5+0.3i$	0	0	−0.4	17.9	−7.7	0	0	0	0	$-0.5+0.2i$	$6.2-0.2i$	$-0.1i$	0	0	0
$\langle\frac{3}{2},-\frac{3}{2}\|$	0	$6.8+0.4i$	$-0.3-0.1i$	0	0	0	10.1	16.0	−0.4	0.1	0	0	0	$6.8-0.4i$	$-0.3+0.1i$	0
$\langle\frac{1}{2},-\frac{1}{2}\|$	0	$-0.5-0.2i$	5.9	0	0	0	16.0	−37.0	20.5	−0.4	0	0	0	$-0.5+0.2i$	5.9	0
$\langle-\frac{1}{2},\frac{1}{2}\|$	0	5.9	$-0.5-0.2i$	0	0	0	−0.4	20.5	−37.0	16.0	0	0	0	5.9	$-0.5+0.2i$	0
$\langle-\frac{3}{2},\frac{3}{2}\|$	0	$-0.3-0.1i$	$6.8+0.4i$	0	0	0	0.1	−0.4	16.0	10.1	0	0	0	$-0.3+0.1i$	$6.8-0.4i$	0
$\langle\frac{1}{2},-\frac{3}{2}\|$	0	0	0	$0.1i$	$6.2+0.2i$	$-0.5-0.2i$	0	0	0	0	−7.7	17.9	−0.4	0	0	$6.5-0.3i$
$\langle-\frac{1}{2},-\frac{1}{2}\|$	0	0	0	$6.2+0.2i$	$-0.9-0.3i$	$6.2+0.2i$	0	0	0	0	17.9	−31.8	17.9	0	0	$-1.0+0.4i$
$\langle-\frac{3}{2},\frac{1}{2}\|$	0	0	0	$-0.5-0.2i$	$6.2+0.2i$	$0.1i$	0	0	0	0	−0.4	17.9	−7.7	0	0	$6.5-0.3i$
$\langle-\frac{1}{2},-\frac{3}{2}\|$	0	0	0	0	0	0	$6.5+0.3i$	$-0.8-0.3i$	$6.2+0.2i$	0	0	0	0	8.0	15.4	0
$\langle-\frac{3}{2},-\frac{1}{2}\|$	0	0	0	0	0	0	0	$6.2+0.2i$	$-0.8-0.3i$	$6.5+0.3i$	0	0	0	15.4	8.0	0
$\langle-\frac{3}{2},-\frac{3}{2}\|$	0	0	0	0	0	0	0	0	0	0	$6.5+0.3i$	$-1.0-0.4i$	$6.5+0.3i$	0	0	58.2

Table S14 Complex 1: Matrix elements of $\hat{H}^{\mathrm{MS}} - \hat{H}^{\mathrm{eff}}$ (cm^{-1}) expressed in the $|M_{Sa}, M_{Sb}\rangle$ uncoupled-spin basis. $\hat{H}^{\mathrm{MS}}$ and the sign-revised $\hat{H}^{\mathrm{eff}}$ are taken from Tables S11 and S13 respectively.

Diff.	$\lvert\frac{3}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},\frac{1}{2}\rangle$	$\lvert\frac{1}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},-\frac{1}{2}\rangle$	$\lvert\frac{1}{2},\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},-\frac{3}{2}\rangle$	$\lvert\frac{1}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},\frac{3}{2}\rangle$	$\lvert\frac{1}{2},-\frac{3}{2}\rangle$	$\lvert-\frac{1}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},-\frac{3}{2}\rangle$	$\lvert-\frac{3}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},-\frac{3}{2}\rangle$
$\langle\frac{3}{2},\frac{3}{2}\rvert$	1.7	−0.1	−0.1	$-0.1+0.3i$	$1.0-0.4i$	$-0.1+0.3i$	0	0	0	0	0	0	0	0	0	0
$\langle\frac{3}{2},\frac{1}{2}\rvert$	−0.1	0.4	1.4	0	0	0	$-0.4+0.4i$	$0.5-0.2i$	0.5	$0.3-0.1i$	0	0	0	0	0	0
$\langle\frac{1}{2},\frac{3}{2}\rvert$	−0.1	1.4	0.4	0	0	0	$0.3-0.1i$	0.5	$0.5-0.2i$	$-0.4+0.4i$	0	0	0	0	0	0
$\langle\frac{3}{2},-\frac{1}{2}\rvert$	$-0.1-0.3i$	0	0	−0.7	1.4	0.4	0	$-0.1i$	0	0	$0.1i$	$0.2+0.1i$	$0.5-0.2i$	0	0	0
$\langle\frac{1}{2},\frac{1}{2}\rvert$	$1.0+0.4i$	0	0	1.4	−0.1	1.4	0	0	0	0	$0.2+0.1i$	$0.9-0.3i$	$0.2+0.1i$	0	0	0
$\langle-\frac{1}{2},\frac{3}{2}\rvert$	$-0.1-0.3i$	0	0	0.4	1.4	−0.7	0	0	$-0.1i$	0	$0.5-0.2i$	$0.2+0.1i$	$0.1i$	0	0	0
$\langle\frac{3}{2},-\frac{3}{2}\rvert$	0	$-0.4-0.4i$	$0.3+0.1i$	$-0.1i$	0	0	−0.5	0.8	0.4	−0.1	$-0.1i$	0	0	$-0.4+0.4i$	$0.3-0.1i$	0
$\langle\frac{1}{2},-\frac{1}{2}\rvert$	0	$0.5+0.2i$	0.5	0	0	0	0.8	−0.5	1.8	0.4	0	0	0	$0.5-0.2i$	0.5	0
$\langle-\frac{1}{2},\frac{1}{2}\rvert$	0	0.5	$0.5+0.2i$	0	0	0	0.4	1.8	−0.5	0.8	0	0	0	0.5	$0.5-0.2i$	0
$\langle-\frac{3}{2},\frac{3}{2}\rvert$	0	$0.3+0.1i$	$-0.4-0.4i$	0	0	$-0.1i$	−0.1	0.4	0.8	−0.5	0	0	$-0.1i$	$0.3-0.1i$	$-0.4+0.4i$	0
$\langle\frac{1}{2},-\frac{3}{2}\rvert$	0	0	0	$-0.1i$	$0.2-0.1i$	$0.5+0.2i$	$0.1i$	0	0	0	−0.7	1.4	0.4	0	0	$-0.1+0.3i$
$\langle-\frac{1}{2},-\frac{1}{2}\rvert$	0	0	0	$0.2-0.1i$	$0.9+0.3i$	$0.2-0.1i$	0	0	0	0	1.4	−0.1	1.4	0	0	$1.0-0.4i$
$\langle-\frac{3}{2},\frac{1}{2}\rvert$	0	0	0	$0.5+0.2i$	$0.2-0.1i$	$-0.1i$	0	0	0	$0.1i$	0.4	1.4	−0.7	0	0	$-0.1+0.3i$
$\langle-\frac{1}{2},-\frac{3}{2}\rvert$	0	0	0	0	0	0	$-0.1-0.2i$	$0.8+0.3i$	$0.2-0.2i$	0	0	0	0	0.4	1.4	0.1
$\langle-\frac{3}{2},-\frac{1}{2}\rvert$	0	0	0	0	0	0	0	$0.2-0.2i$	$0.8+0.3i$	$-0.1-0.2i$	0	0	0	1.4	0.4	0.1
$\langle-\frac{3}{2},-\frac{3}{2}\rvert$	0	0	0	0	0	0	0	0	0	0	$-0.1-0.3i$	$1.0+0.4i$	$-0.1-0.3i$	0.1	0.1	1.7

Table S15 Complex 1: Matrix elements of $\hat{H}^{\mathrm{MS}} - \hat{H}^{\mathrm{eff}}$ (cm^{-1}) expressed in the $|S, M_S\rangle$ coupled-spin basis. The $\hat{H}^{\mathrm{MS}}$ and $\hat{H}^{\mathrm{eff}}$ matrices are taken from Tables S10 and S12 respectively.

Diff.	$\lvert3,3\rangle$	$\lvert3,2\rangle$	$\lvert3,1\rangle$	$\lvert3,0\rangle$	$\lvert3,-1\rangle$	$\lvert3,-2\rangle$	$\lvert3,-3\rangle$	$\lvert2,2\rangle$	$\lvert2,1\rangle$	$\lvert2,0\rangle$	$\lvert2,-1\rangle$	$\lvert2,-2\rangle$	$\lvert1,1\rangle$	$\lvert1,0\rangle$	$\lvert1,-1\rangle$	$\lvert0,0\rangle$
$\langle3,3\rvert$	1.7	−0.1	0.7	0	0	0	0	0	0	0	0	0	$-0.8+0.5i$	0	0	0
$\langle3,2\rvert$	−0.1	1.8	−0.1	0.9	0	0	0	0	0	0	0	0	0	$-0.4+0.3i$	0	0
$\langle3,1\rvert$	0.7	−0.1	1.8	0	1.0	0	0	0	0	0	0	0	0.3	0	$-0.2+0.1i$	0
$\langle3,0\rvert$	0	0.9	0	1.8	0	0.9	0	0	0	0	0	0	0	0.4	0	0
$\langle3,-1\rvert$	0	0	1.0	0	1.8	0.1	0.7	0	0	0	0	0	$-0.2-0.1i$	0	0.3	0
$\langle3,-2\rvert$	0	0	0	0.9	0.1	1.8	0.1	0	0	0	0	0	0	$-0.4-0.3i$	0	0
$\langle3,-3\rvert$	0	0	0	0	0.7	0.1	1.7	0	0	0	0	0	0	0	$-0.8-0.5i$	0
$\langle2,2\rvert$	0	0	0	0	0	0	0	−1.0	$0.1i$	$-0.4+0.2i$	0	0	0	0	0	$-0.5+0.5i$
$\langle2,1\rvert$	0	0	0	0	0	0	0	$-0.1i$	−1.1	0	$-0.5+0.3i$	0	0	0	0	$0.1i$
$\langle2,0\rvert$	0	0	0	0	0	0	0	$-0.4-0.2i$	0	−1.1	0	$-0.4+0.2i$	0	0	0	1.0
$\langle2,-1\rvert$	0	0	0	0	0	0	0	0	$-0.5-0.3i$	0	−1.1	$-0.1i$	0	0	0	$0.1i$
$\langle2,-2\rvert$	0	0	0	0	0	0	0	0	0	$0.4+0.2i$	$0.1i$	−1.0	0	0	0	$-0.5-0.5i$
$\langle1,1\rvert$	$-0.8-0.5i$	0	0.3	0	$-0.2+0.1i$	0	0	0	0	0	0	0	−2.2	$0.1i$	$0.4-0.4i$	0
$\langle1,0\rvert$	0	$-0.4-0.3i$	0	0.4	0	$-0.4+0.3i$	0	0	0	0	0	0	$-0.1i$	−1.1	$-0.1i$	0
$\langle1,-1\rvert$	0	0	$-0.2-0.1i$	0	0.3	0	$-0.8+0.5i$	0	0	0	0	0	$0.4+0.4i$	$0.1i$	−2.2	0
$\langle0,0\rvert$	0	0	0	0	0	0	0	$-0.5-0.5i$	$-0.1i$	1.0	$-0.1i$	$-0.5+0.5i$	0	0	0	−1.7

Table S16 Complex 1: Matrix elements of $\hat{H}^{\mathrm{MS}} = J\hat{S}_a\hat{S}_b + \hat{S}_a\bar{\bar{D}}_a\hat{S}_a + \hat{S}_b\bar{\bar{D}}_b\hat{S}_b + \hat{S}_a\bar{\bar{D}}_{ab}\hat{S}_b$ expressed in the $|M_{Sa}, M_{Sb}\rangle$ uncoupled-spin basis.

Diff.	$\|\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{3}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},-\frac{3}{2}\rangle$
$\langle\frac{3}{2},\frac{3}{2}\|$	58.2	0	0	6.4	−0.5	6.4	0	0	0	0	0	0	0	0	0	0
$\langle\frac{3}{2},\frac{1}{2}\|$	0	8.0	15.6	0	0	0	6.4	−0.6	6.4	0	0	0	0	0	0	0
$\langle\frac{1}{2},\frac{3}{2}\|$	0	15.6	8.0	0	0	0	0	6.4	−0.6	6.4	0	0	0	0	0	0
$\langle\frac{3}{2},-\frac{1}{2}\|$	6.4	0	0	−8.0	18.0	0	0	0	0	0	−0.5	6.4	0	0	0	0
$\langle\frac{1}{2},\frac{1}{2}\|$	−0.5	0	0	18.0	−31.6	18.0	0	0	0	0	6.4	−0.7	6.4	0	0	0
$\langle-\frac{1}{2},\frac{3}{2}\|$	6.4	0	0	0	18.0	−8.0	0	0	0	0	0	6.4	−0.5	0	0	0
$\langle\frac{3}{2},-\frac{3}{2}\|$	0	6.4	0	0	0	0	10.3	15.6	0	0	0	0	0	6.4	0	0
$\langle\frac{1}{2},-\frac{1}{2}\|$	0	−0.6	6.4	0	0	0	15.6	−36.9	20.3	0	0	0	0	−0.6	6.4	0
$\langle-\frac{1}{2},\frac{1}{2}\|$	0	6.4	−0.6	0	0	0	0	20.3	−36.9	15.6	0	0	0	6.4	−0.6	0
$\langle-\frac{3}{2},\frac{1}{2}\|$	0	0	6.4	0	0	0	0	0	15.6	10.3	0	0	0	0	6.4	0
$\langle\frac{1}{2},-\frac{3}{2}\|$	0	0	0	−0.5	6.4	0	0	0	0	0	−8.0	18.0	0	0	0	6.4
$\langle-\frac{1}{2},-\frac{1}{2}\|$	0	0	0	6.4	−0.7	6.4	0	0	0	0	18.0	−31.6	18.0	0	0	−0.5
$\langle-\frac{3}{2},\frac{1}{2}\|$	0	0	0	0	6.4	−0.5	0	0	0	0	0	18.0	−8.0	0	0	6.4
$\langle-\frac{1}{2},-\frac{3}{2}\|$	0	0	0	0	0	0	6.4	−0.6	6.4	0	0	0	0	8.0	15.6	0
$\langle-\frac{3}{2},-\frac{1}{2}\|$	0	0	0	0	0	0	0	6.4	−0.6	6.4	0	0	0	15.6	8.0	0
$\langle-\frac{3}{2},-\frac{3}{2}\|$	0	0	0	0	0	0	0	0	0	0	6.4	−0.5	6.4	0	0	58.2

Table S17 Complex 1: Matrix elements of $\hat{H}^{\mathrm{MS}} = J\hat{S}_a\hat{S}_b + \hat{S}_a\bar{\bar{D}}_a\hat{S}_a + \hat{S}_b\bar{\bar{D}}_b\hat{S}_b + \hat{S}_a\bar{\bar{D}}_{ab}\hat{S}_b$ expressed in the $|S, M_S\rangle$ coupled-spin basis.

Diff.	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle3,3\|$	58.2	0	5.3	0	0	0	0	0	0	0	0	0	7.3	0	0	0
$\langle3,2\|$	0	23.6	0	7.5	0	0	0	0	0	0	0	0	0	4.2	0	0
$\langle3,1\|$	5.3	0	2.8	0	8.2	0	0	0	0	0	0	0	16.7	0	1.9	0
$\langle3,0\|$	0	7.5	0	−4.6	0	7.5	0	0	0	0	0	0	0	20.6	0	0
$\langle3,-1\|$	0	0	8.2	0	2.8	0	5.3	0	0	0	0	0	1.9	0	16.7	0
$\langle3,-2\|$	0	0	0	7.5	0	23.6	0	0	0	0	0	0	0	4.2	0	0
$\langle3,-3\|$	0	0	0	0	5.3	0	58.2	0	0	0	0	0	0	0	7.3	0
$\langle2,2\|$	0	0	0	0	0	0	0	−7.6	0	−0.4	0	0	0	0	0	9.4
$\langle2,1\|$	0	0	0	0	0	0	0	0	−8.0	0	−0.5	0	0	0	0	0
$\langle2,0\|$	0	0	0	0	0	0	0	−0.4	0	−7.9	0	−0.4	0	0	0	33.8
$\langle2,-1\|$	0	0	0	0	0	0	0	0	−0.5	0	−8.0	0	0	0	0	0
$\langle2,-2\|$	0	0	0	0	0	0	0	0	0	−0.4	0	−7.6	0	0	0	9.4
$\langle1,1\|$	7.3	0	16.7	0	1.9	0	0	0	0	0	0	0	−42.4	0	−9.4	0
$\langle1,0\|$	0	4.2	0	20.6	0	4.2	0	0	0	0	0	0	0	−1.7	0	0
$\langle1,-1\|$	0	0	1.9	0	16.7	0	7.3	0	0	0	0	0	−9.4	0	−42.4	0
$\langle0,0\|$	0	0	0	0	0	0	0	9.4	0	33.8	0	9.4	0	0	0	−39.0

Table S18 Complex 1: Difference between the numerical matrix elements of $\hat{H}^{\mathrm{MS}} = J\hat{S}_a\hat{S}_b + \hat{S}_a\bar{\bar{D}}_a\hat{S}_a + \hat{S}_b\bar{\bar{D}}_b\hat{S}_b + \hat{S}_a\bar{\bar{D}}_{ab}\hat{S}_b$ (Table S16) and $\hat{H}^{\mathrm{eff}}$ (Table S13) expressed in the $|M_{Sa},M_{Sb}\rangle$ uncoupled-spin basis.

Diff.	$\lvert\frac{3}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},\frac{1}{2}\rangle$	$\lvert\frac{1}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},-\frac{1}{2}\rangle$	$\lvert\frac{1}{2},\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},-\frac{3}{2}\rangle$	$\lvert\frac{1}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},\frac{3}{2}\rangle$	$\lvert\frac{1}{2},-\frac{3}{2}\rangle$	$\lvert-\frac{1}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},-\frac{3}{2}\rangle$	$\lvert-\frac{3}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},-\frac{3}{2}\rangle$
$\langle\frac{3}{2},\frac{3}{2}\rvert$	0	0	0	$-0.1+0.3i$	$0.5-0.4i$	$-0.1+0.3i$	0	0	0	0	0	0	0	0	0	0
$\langle\frac{3}{2},\frac{1}{2}\rvert$	0	0	0.2	0	0	0	$-0.4+0.4i$	$-0.1-0.2i$	0.4	$0.3-0.1i$	0	0	0	0	0	0
$\langle\frac{1}{2},\frac{3}{2}\rvert$	0	0.2	0	0	0	0	$0.3-0.1i$	0.4	$-0.1-0.2i$	$-0.4+0.4i$	0	0	0	0	0	0
$\langle\frac{3}{2},-\frac{1}{2}\rvert$	$-0.1-0.3i$	0	0	-0.3	0.1	0.4	0	0	0	0	$-0.5+0.1i$	$0.1+0.2i$	$0.5-0.2i$	0	0	0
$\langle\frac{1}{2},\frac{1}{2}\rvert$	$0.5+0.4i$	0	0	0.1	0.2	0.1	0	0	0	0	$0.1+0.2i$	$0.3-0.3i$	$0.1+0.2i$	0	0	0
$\langle-\frac{1}{2},\frac{3}{2}\rvert$	$-0.1-0.3i$	0	0	0.4	0.1	-0.3	0	0	0	0	$0.5-0.2i$	$0.1+0.2i$	$-0.5+0.1i$	0	0	0
$\langle\frac{3}{2},-\frac{3}{2}\rvert$	0	$-0.4-0.4i$	$0.3+0.1i$	0	0	0	0.2	-0.4	0.4	-0.1	0	0	0	$-0.4+0.4i$	$0.3-0.1i$	0
$\langle\frac{1}{2},-\frac{1}{2}\rvert$	0	$-0.1+0.2i$	0.4	0	0	0	-0.4	0	-0.2	0.4	0	0	0	$-0.1-0.2i$	0.4	0
$\langle-\frac{1}{2},\frac{1}{2}\rvert$	0	0.4	$-0.1+0.2i$	0	0	0	0.4	-0.2	0	-0.4	0	0	0	0.4	$-0.1-0.2i$	0
$\langle-\frac{3}{2},\frac{3}{2}\rvert$	0	$0.3+0.1i$	$-0.4-0.4i$	0	0	0	-0.1	0.4	-0.4	0.2	0	0	0	$0.3-0.1i$	$-0.4+0.4i$	0
$\langle\frac{1}{2},-\frac{3}{2}\rvert$	0	0	0	$-0.5-0.1i$	$0.1-0.2i$	$0.5+0.2i$	0	0	0	0	-0.3	0.1	0.4	0	0	$-0.1+0.3i$
$\langle-\frac{1}{2},-\frac{1}{2}\rvert$	0	0	0	$0.1-0.2i$	$0.3+0.3i$	$0.1-0.2i$	0	0	0	0	0.1	0.2	0.1	0	0	$0.5-0.4i$
$\langle-\frac{3}{2},\frac{1}{2}\rvert$	0	0	0	$0.5+0.2i$	$0.1-0.2i$	$-0.5-0.1i$	0	0	0	0	0.4	0.1	-0.3	0	0	$-0.1+0.3i$
$\langle-\frac{1}{2},-\frac{3}{2}\rvert$	0	0	0	0	0	0	$-0.1-0.3i$	$0.2+0.3i$	$0.1-0.2i$	0	0	0	0	0	0.2	0
$\langle-\frac{3}{2},-\frac{1}{2}\rvert$	0	0	0	0	0	0	0	$0.1-0.2i$	$0.2+0.3i$	$-0.1-0.3i$	0	0	0	0.2	0	0
$\langle-\frac{3}{2},-\frac{3}{2}\rvert$	0	0	0	0	0	0	0	0	0	0	$-0.1-0.3i$	$0.5+0.4i$	$-0.1-0.3i$	0	0	0

Table S19 Complex 1: Difference between the numerical matrix elements of $\hat{H}^{\mathrm{MS}} = J\hat{S}_a\hat{S}_b + \hat{S}_a\bar{\bar{D}}_a\hat{S}_a + \hat{S}_b\bar{\bar{D}}_b\hat{S}_b + \hat{S}_a\bar{\bar{D}}_{ab}\hat{S}_b$ (Table S17) and $\hat{H}^{\mathrm{eff}}$ (Table S12) expressed in the $|S,M_S\rangle$ coupled-spin basis.

Diff.	$\lvert3,3\rangle$	$\lvert3,2\rangle$	$\lvert3,1\rangle$	$\lvert3,0\rangle$	$\lvert3,-1\rangle$	$\lvert3,-2\rangle$	$\lvert3,-3\rangle$	$\lvert2,2\rangle$	$\lvert2,1\rangle$	$\lvert2,0\rangle$	$\lvert2,-1\rangle$	$\lvert2,-2\rangle$	$\lvert1,1\rangle$	$\lvert1,0\rangle$	$\lvert1,-1\rangle$	$\lvert0,0\rangle$
$\langle3,3\rvert$	0	0	0.2	0	0	0	0	0	0	0	0	0	$-0.5+0.6i$	0	0	0
$\langle3,2\rvert$	0	0.3	0	0.3	0	0	0	0	0	0	0	0	0	$-0.2+0.3i$	0	0
$\langle3,1\rvert$	0.2	0	0.3	0	0.3	0	0	0	0	0	0	0	0	0	$-0.1+0.1i$	0
$\langle3,0\rvert$	0	0.3	0	-0.1	0	0.3	0	0	0	0	0	0	0	0.1	0	0
$\langle3,-1\rvert$	0	0	0.3	0	0.3	0	0.2	0	0	0	0	0	$-0.1-0.1i$	0	0	0
$\langle3,-2\rvert$	0	0	0	0.3	0	0.3	0	0	0	0	0	0	0	$-0.2-0.3i$	0	0
$\langle3,-3\rvert$	0	0	0	0	0.2	0	0	0	0	0	0	0	0	0	$-0.5-0.6i$	0
$\langle2,2\rvert$	0	0	0	0	0	0	0	-0.2	$0.1i$	$-0.9+0.2i$	0	0	0	0	0	$-0.2+0.5i$
$\langle2,1\rvert$	0	0	0	0	0	0	0	$-0.1i$	-0.7	0	$-1.0+0.3i$	0	0	0	0	$-0.1+0.1i$
$\langle2,0\rvert$	0	0	0	0	0	0	0	$-0.9-0.2i$	0	-0.6	0	$-0.9+0.2i$	0	0	0	0
$\langle2,-1\rvert$	0	0	0	0	0	0	0	0	$-1.0-0.3i$	0	-0.7	$-0.1i$	0	0	0	$0.1+0.1i$
$\langle2,-2\rvert$	0	0	0	0	0	0	0	0	0	$0.2i$	$0.1i$	-0.2	0	0	0	$-0.2-0.5i$
$\langle1,1\rvert$	$-0.5-0.6i$	0	0	0	$-0.1+0.1i$	0	0	0	0	0	0	0	0	-0.1	$-0.1-0.4i$	0
$\langle1,0\rvert$	0	$-0.2-0.3i$	0	0.1	0	$-0.2+0.3i$	0	0	0	0	0	0	-0.1	0.1	0.1	0
$\langle1,-1\rvert$	0	0	$-0.1-0.1i$	0	0	0	$-0.5+0.6i$	0	0	0	0	0	$-0.1+0.4i$	0.1	0	0
$\langle0,0\rvert$	0	0	0	0	0	0	0	$-0.2-0.5i$	$-0.1-0.1i$	0	$0.1-0.1i$	$-0.2+0.5i$	0	0	0	1.1

Table S20 Analytical matrix elements of $\hat{H}^{\mathrm{zee}} = \mu_{\mathrm{B}}\vec{B}\hat{g}_a\hat{S}_a$ expressed in the $|M_{Sa}, M_{Sb}\rangle$ uncoupled-spin basis.[a]

$\mu_{\mathrm{B}}\vec{B}\hat{g}_a\hat{S}_a$	$\lvert\frac{3}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},\frac{1}{2}\rangle$	$\lvert\frac{1}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},-\frac{1}{2}\rangle$	$\lvert\frac{1}{2},\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},-\frac{3}{2}\rangle$	$\lvert\frac{1}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},\frac{3}{2}\rangle$	$\lvert\frac{1}{2},-\frac{3}{2}\rangle$	$\lvert-\frac{1}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},-\frac{3}{2}\rangle$	$\lvert-\frac{3}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},-\frac{3}{2}\rangle$
$\langle\frac{3}{2},\frac{3}{2}\rvert$	$-X$	0	Y	0	0	0	0	0	0	0	0	0	0	0	0	0
$\langle\frac{3}{2},\frac{1}{2}\rvert$	0	$-X$	0	0	Y	0	0	0	0	0	0	0	0	0	0	0
$\langle\frac{1}{2},\frac{3}{2}\rvert$	Y^*	0	$-Z$	0	0	T	0	0	0	0	0	0	0	0	0	0
$\langle\frac{3}{2},-\frac{1}{2}\rvert$	0	0	0	$-X$	0	0	0	Y	0	0	0	0	0	0	0	0
$\langle\frac{1}{2},\frac{1}{2}\rvert$	0	Y^*	0	0	$-Z$	0	0	0	T	0	0	0	0	0	0	0
$\langle-\frac{1}{2},\frac{3}{2}\rvert$	0	0	T^*	0	0	Z	0	0	0	Y	0	0	0	0	0	0
$\langle\frac{3}{2},-\frac{3}{2}\rvert$	0	0	0	0	0	0	$-X$	0	0	0	Y	0	0	0	0	0
$\langle\frac{1}{2},-\frac{1}{2}\rvert$	0	0	0	Y^*	0	0	0	$-Z$	0	0	0	T	0	0	0	0
$\langle-\frac{1}{2},\frac{1}{2}\rvert$	0	0	0	0	T^*	0	0	0	Z	0	0	0	Y	0	0	0
$\langle-\frac{3}{2},\frac{3}{2}\rvert$	0	0	0	0	0	Y^*	0	0	0	X	0	0	0	0	0	0
$\langle\frac{1}{2},-\frac{3}{2}\rvert$	0	0	0	0	0	0	Y^*	0	0	0	$-Z$	0	0	T	0	0
$\langle-\frac{1}{2},-\frac{1}{2}\rvert$	0	0	0	0	0	0	0	T^*	0	0	0	Z	0	0	Y	0
$\langle-\frac{3}{2},\frac{1}{2}\rvert$	0	0	0	0	0	0	0	0	Y^*	0	0	0	X	0	0	0
$\langle-\frac{1}{2},-\frac{3}{2}\rvert$	0	0	0	0	0	0	0	0	0	0	T^*	0	0	Z	0	Y
$\langle-\frac{3}{2},-\frac{1}{2}\rvert$	0	0	0	0	0	0	0	0	0	0	0	Y^*	0	0	X	0
$\langle-\frac{3}{2},-\frac{3}{2}\rvert$	0	0	0	0	0	0	0	0	0	0	0	0	0	Y^*	0	X

[a]Legend:
$X = -\frac{3}{2}\mu_{\mathrm{B}}\left(B_x g^a_{xz} + B_y g^a_{yz} + B_z g^a_{zz}\right)$; $Y = \frac{\sqrt{3}}{2}\mu_{\mathrm{B}}\left[\left(B_x g^a_{xx} + B_y g^a_{yx} + B_z g^a_{zx}\right) - i\left(B_x g^a_{xy} + B_y g^a_{yy} + B_z g^a_{zy}\right)\right]$
$Z = -\frac{1}{2}\mu_{\mathrm{B}}\left(B_x g^a_{xz} + B_y g^a_{yz} + B_z g^a_{zz}\right)$; $T = \mu_{\mathrm{B}}\left[\left(B_x g^a_{xx} + B_y g^a_{yx} + B_z g^a_{zx}\right) - i\left(B_x g^a_{xy} + B_y g^a_{yy} + B_z g^a_{zy}\right)\right]$; the asterix stands for complex conjugate.

Table S21 Analytical matrix elements of $\hat{H}^{\mathrm{zee}} = \mu_{\mathrm{B}}\vec{B}\hat{g}_b\hat{S}_b$ expressed in the $|M_{Sa}, M_{Sb}\rangle$ uncoupled-spin basis.[a]

$\mu_{\mathrm{B}}\vec{B}\hat{g}_b\hat{S}_b$	$\lvert\frac{3}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},\frac{1}{2}\rangle$	$\lvert\frac{1}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},-\frac{1}{2}\rangle$	$\lvert\frac{1}{2},\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},\frac{3}{2}\rangle$	$\lvert\frac{3}{2},-\frac{3}{2}\rangle$	$\lvert\frac{1}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},\frac{3}{2}\rangle$	$\lvert\frac{1}{2},-\frac{3}{2}\rangle$	$\lvert-\frac{1}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},\frac{1}{2}\rangle$	$\lvert-\frac{1}{2},-\frac{3}{2}\rangle$	$\lvert-\frac{3}{2},-\frac{1}{2}\rangle$	$\lvert-\frac{3}{2},-\frac{3}{2}\rangle$
$\langle\frac{3}{2},\frac{3}{2}\rvert$	$-X$	Y	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\langle\frac{3}{2},\frac{1}{2}\rvert$	Y^*	$-Z$	0	T	0	0	0	0	0	0	0	0	0	0	0	0
$\langle\frac{1}{2},\frac{3}{2}\rvert$	0	0	$-X$	0	Y	0	0	0	0	0	0	0	0	0	0	0
$\langle\frac{3}{2},-\frac{1}{2}\rvert$	0	T^*	0	Z	0	0	Y	0	0	0	0	0	0	0	0	0
$\langle\frac{1}{2},\frac{1}{2}\rvert$	0	0	Y^*	0	$-Z$	0	0	T	0	0	0	0	0	0	0	0
$\langle-\frac{1}{2},\frac{3}{2}\rvert$	0	0	0	0	0	$-X$	0	0	Y	0	0	0	0	0	0	0
$\langle\frac{3}{2},-\frac{3}{2}\rvert$	0	0	0	Y^*	0	0	X	0	0	0	0	0	0	0	0	0
$\langle\frac{1}{2},-\frac{1}{2}\rvert$	0	0	0	0	T^*	0	0	Z	0	0	Y	0	0	0	0	0
$\langle-\frac{1}{2},\frac{1}{2}\rvert$	0	0	0	0	0	Y^*	0	0	$-Z$	0	0	T	0	0	0	0
$\langle-\frac{3}{2},\frac{3}{2}\rvert$	0	0	0	0	0	0	0	0	0	$-X$	0	0	Y	0	0	0
$\langle\frac{1}{2},-\frac{3}{2}\rvert$	0	0	0	0	0	0	0	Y^*	0	0	X	0	0	0	0	0
$\langle-\frac{1}{2},-\frac{1}{2}\rvert$	0	0	0	0	0	0	0	0	T^*	0	0	Z	0	Y	0	0
$\langle-\frac{3}{2},\frac{1}{2}\rvert$	0	0	0	0	0	0	0	0	0	Y^*	0	0	$-Z$	0	T	0
$\langle-\frac{1}{2},-\frac{3}{2}\rvert$	0	0	0	0	0	0	0	0	0	0	0	Y^*	0	X	0	0
$\langle-\frac{3}{2},-\frac{1}{2}\rvert$	0	0	0	0	0	0	0	0	0	0	0	0	T^*	0	Z	Y
$\langle-\frac{3}{2},-\frac{3}{2}\rvert$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Y^*	X

[a]Legend:
$X = -\frac{3}{2}\mu_{\mathrm{B}}\left(B_x g^b_{xz} + B_y g^b_{yz} + B_z g^b_{zz}\right)$; $Y = \frac{\sqrt{3}}{2}\mu_{\mathrm{B}}\left[\left(B_x g^b_{xx} + B_y g^b_{yx} + B_z g^b_{zx}\right) - i\left(B_x g^b_{xy} + B_y g^b_{yy} + B_z g^b_{zy}\right)\right]$
$Z = -\frac{1}{2}\mu_{\mathrm{B}}\left(B_x g^b_{xz} + B_y g^b_{yz} + B_z g^b_{zz}\right)$; $T = \mu_{\mathrm{B}}\left[\left(B_x g^b_{xx} + B_y g^b_{yx} + B_z g^b_{zx}\right) - i\left(B_x g^b_{xy} + B_y g^b_{yy} + B_z g^b_{zy}\right)\right]$; the asterix stands for complex conjugate.

Table S22 SOCI energies, in cm^{-1}, corresponding to the 16 low-lying spin-orbit states of complex 2, calculated with various approaches.

State idx	SO-CASSCF	SO-NEVPT2	model//SO-NEVPT2
ψ_1	0.0	0.0	0.0
ψ_2	1.9	1.9	2.1
ψ_3	3.9	3.6	3.9
ψ_4	8.7	7.7	8.1
ψ_5	214.6	177.0	178.7
ψ_6	215.2	177.7	179.3
ψ_7	218.9	180.6	182.2
ψ_8	220.2	182.2	183.7
ψ_9	238.0	206.4	206.6
ψ_{10}	238.3	206.9	207.1
ψ_{11}	241.4	209.6	210.4
ψ_{12}	243.8	212.2	212.9
ψ_{13}	448.8	379.7	382.3
ψ_{14}	449.0	380.0	382.4
ψ_{15}	457.8	388.4	390.5
ψ_{16}	458.2	389.0	391.2

Table S23 Contribution of the $|S,M_S\rangle$ components of the low-lying $S = 3$, 2, 1, 0 states to the wavefunctions of the 16 low-energy spin-orbit states, obtained in SO-NEVPT2 calculations on complex 2 in an arbitrary *xyz* frame.[a]

SOCI state	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
ψ_1	0.1	0.04	0.04	0.07	0.04	0.04	0.1	0.01	0.02	0	0.02	0.01	0.02	0	0.02	0
ψ_2	0.05	0.06	0.05	0.04	0.05	0.06	0.05	0.01	0	0.05	0	0.01	0.03	0.06	0.03	0
ψ_3	0.07	0.02	0.02	0.01	0.02	0.02	0.07	0.02	0.01	0.02	0.01	0.02	0.07	0.04	0.07	0.02
ψ_4	0	0	0.01	0.01	0.01	0	0	0.09	0.02	0.01	0.02	0.09	0.01	0.06	0.01	0.17
ψ_5	0.02	0.15	0.02	0.05	0.02	0.15	0.02	0.02	0.02	0.12	0.02	0.02	0.01	0	0.01	0
ψ_6	0.06	0.01	0.1	0.05	0.1	0.01	0.06	0.02	0.08	0	0.08	0.02	0	0.02	0	0.02
ψ_7	0.04	0.04	0.02	0	0.02	0.04	0.04	0.02	0.08	0.04	0.08	0.02	0.09	0	0.09	0.01
ψ_8	0.01	0.01	0.02	0.03	0.02	0.01	0.01	0.1	0.04	0.01	0.04	0.1	0.03	0.14	0.03	0.05
ψ_9	0.06	0.09	0	0.06	0	0.09	0.06	0.03	0.05	0.13	0.05	0.03	0	0	0	0
ψ_{10}	0.06	0.05	0.07	0.01	0.07	0.05	0.06	0.02	0.09	0.08	0.09	0.02	0	0.01	0	0
ψ_{11}	0.04	0.02	0.03	0	0.03	0.02	0.04	0.03	0.11	0.04	0.11	0.03	0.05	0.01	0.05	0.05
ψ_{12}	0.01	0	0.01	0.01	0.01	0	0.01	0.09	0.03	0.02	0.03	0.09	0.06	0.23	0.06	0.02
ψ_{13}	0.05	0.02	0.27	0.02	0.27	0.02	0.05	0.03	0.02	0.01	0.02	0.03	0	0	0	0
ψ_{14}	0.02	0.14	0.02	0.35	0.02	0.14	0.02	0.02	0.03	0.01	0.03	0.02	0	0	0	0
ψ_{15}	0.02	0.01	0.01	0	0.01	0.01	0.02	0.11	0.02	0.09	0.02	0.11	0.04	0.05	0.04	0.26
ψ_{16}	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.04	0.03	0.02	0.03	0.04	0.27	0	0.27	0.05

[a]The corresponding state energies are printed in Table S22.

Table S24 Contribution of the $|S,M_S\rangle$ components of the low-lying $S = 3$, 2, 1, 0 states to the wavefunctions of the 16 low-energy spin-orbit states, obtained in SO-NEVPT2 calculations on complex 2 in the molecular PAF.

SOCI state	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
ψ_1	0	0	0	0.42	0	0	0	0.01	0.02	0	0.02	0.01	0	0.04	0	0
ψ_2	0	0	0.17	0	0.17	0	0	0.02	0.01	0.01	0.01	0.02	0.05	0	0.05	0
ψ_3	0	0	0.12	0	0.12	0	0	0.02	0.01	0.01	0.01	0.02	0.09	0	0.09	0.01
ψ_4	0	0.01	0	0	0	0.01	0	0	0	0.23	0	0	0.04	0	0.04	0.17
ψ_5	0.01	0.19	0.01	0.01	0.01	0.19	0.01	0.09	0	0	0	0.09	0	0.01	0	0
ψ_6	0.02	0.16	0.02	0	0.02	0.16	0.02	0.09	0.01	0	0.01	0.09	0.01	0	0.01	0.02
ψ_7	0.01	0.01	0.07	0.01	0.07	0.01	0.01	0.01	0.11	0	0.11	0.01	0.08	0.04	0.08	0.01
ψ_8	0.01	0	0.03	0	0.03	0	0.01	0.01	0.14	0	0.14	0.01	0.09	0	0.09	0.05
ψ_9	0.02	0.12	0.03	0.02	0.03	0.12	0.02	0.14	0.01	0	0.01	0.14	0	0	0	0
ψ_{10}	0.02	0.11	0.03	0.02	0.03	0.11	0.02	0.13	0.02	0.01	0.02	0.13	0.01	0	0.01	0
ψ_{11}	0	0.02	0.07	0	0.07	0.02	0	0.04	0.11	0	0.11	0.04	0.05	0.02	0.05	0.05
ψ_{12}	0	0	0.02	0	0.02	0	0	0	0.13	0	0.13	0	0.16	0.02	0.16	0.02
ψ_{13}	0.35	0	0	0	0	0	0.35	0.03	0.02	0	0.02	0.03	0	0	0	0
ψ_{14}	0.35	0	0	0	0	0	0.35	0.03	0.02	0	0.02	0.03	0	0	0	0
ψ_{15}	0	0.02	0.01	0.01	0.01	0.02	0	0	0	0.34	0	0	0.01	0.1	0.01	0.26
ψ_{16}	0	0	0	0.06	0	0	0	0.02	0.03	0.06	0.03	0.02	0.01	0.52	0.01	0.05

[a]The corresponding state energies are printed in Table S22.

Table S25 Complex 2: Numerical matrix elements (cm^{-1}) of $\hat{H}^{MS}=J\hat{S}_a\hat{S}_b+\hat{S}_a\bar{\bar{D}}_a\hat{S}_a+\hat{S}_b\bar{\bar{D}}_b\hat{S}_b$ expressed in the $|M_{Sa},M_{Sb}\rangle$ uncoupled-spin basis, obtained with the spin-free NEVPT2 $J=-2.85$ cm^{-1} and the calculated local anisotropy tensors shown in Equation **??** of the main manuscript.

$\hat{H}^{MS}$	$\|\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{3}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},-\frac{3}{2}\rangle$
$\langle\frac{3}{2},\frac{3}{2}\|$	155.9	$28.3+25.3i$	$-27.5-24.7i$	$45.1+10.8i$	0	$-11.9-12.5i$	0	0	0	0	0	0	0	0	0	0
$\langle\frac{3}{2},\frac{1}{2}\|$	$28.3-25.3i$	-6.8	-4.3	0	$-27.5-24.7i$	0	$45.1+10.8i$	0	$-11.9-12.5i$	0	0	0	0	0	0	0
$\langle\frac{1}{2},\frac{3}{2}\|$	$-27.5+24.7i$	-4.3	2.5	0	$28.3+25.3i$	0	0	$45.1+10.8i$	0	$-11.9-12.5i$	0	0	0	0	0	0
$\langle\frac{3}{2},-\frac{1}{2}\|$	$45.1-10.8i$	0	0	-2.5	-4.9	0	$-28.3-25.3i$	$-27.5-24.7i$	0	0	0	$-11.9-12.5i$	0	0	0	0
$\langle\frac{1}{2},\frac{1}{2}\|$	0	$-27.5+24.7i$	$28.3-25.3i$	-4.9	-163.0	-4.9	0	0	0	0	$45.1+10.8i$	0	$-11.9-12.5i$	0	0	0
$\langle-\frac{1}{2},\frac{3}{2}\|$	$-11.9+12.5i$	0	0	0	-4.9	6.8	0	0	$28.3+25.3i$	$27.5+24.7i$	0	$45.1+10.8i$	0	0	0	0
$\langle\frac{3}{2},-\frac{3}{2}\|$	0	$45.1-10.8i$	0	$-28.3+25.3i$	0	0	168.7	-4.3	0	0	$-27.5-24.7i$	0	0	$-11.9-12.5i$	0	0
$\langle\frac{1}{2},-\frac{1}{2}\|$	0	0	$45.1-10.8i$	$-27.5+24.7i$	0	0	-4.3	-161.6	-5.7	0	$-28.3-25.3i$	0	0	0	$-11.9-12.5i$	0
$\langle-\frac{1}{2},\frac{1}{2}\|$	0	$-11.9+12.5i$	0	0	0	$28.3-25.3i$	0	-5.7	-161.6	-4.3	0	0	$27.5+24.7i$	$45.1+10.8i$	0	0
$\langle-\frac{3}{2},\frac{3}{2}\|$	0	0	$-11.9+12.5i$	0	0	$27.5-24.7i$	0	0	-4.3	168.7	0	0	$28.3+25.3i$	0	$45.1+10.8i$	0
$\langle\frac{1}{2},-\frac{3}{2}\|$	0	0	0	0	$45.1-10.8i$	0	$-27.5+24.7i$	$-28.3+25.3i$	0	0	6.8	-4.9	0	0	0	$-11.9-12.5i$
$\langle-\frac{1}{2},-\frac{1}{2}\|$	0	0	0	$-11.9+12.5i$	0	$45.1-10.8i$	0	0	0	0	-4.9	-163.0	-4.9	$-28.3-25.3i$	$27.5+24.7i$	0
$\langle-\frac{3}{2},\frac{1}{2}\|$	0	0	0	0	$-11.9+12.5i$	0	0	0	$27.5-24.7i$	$28.3-25.3i$	0	-4.9	-2.5	0	0	$45.1+10.8i$
$\langle-\frac{1}{2},-\frac{3}{2}\|$	0	0	0	0	0	$-11.9+12.5i$	0	$45.1-10.8i$	0	0	$-28.3+25.3i$	0	2.5	-4.3	$27.5+24.7i$	
$\langle-\frac{3}{2},-\frac{1}{2}\|$	0	0	0	0	0	0	$-11.9+12.5i$	0	$45.1-10.8i$	0	$27.5-24.7i$	0	-4.3	-6.8	$-28.3-25.3i$	
$\langle-\frac{3}{2},-\frac{3}{2}\|$	0	0	0	0	0	0	0	0	0	$-11.9+12.5i$	0	$45.1-10.8i$	$27.5-24.7i$	$-28.3+25.3i$	155.9	

Table S26 Complex 2: Numerical matrix elements (cm^{-1}) of $\hat{H}^{MS}=J\hat{S}_a\hat{S}_b+\hat{S}_a\bar{\bar{D}}_a\hat{S}_a+\hat{S}_b\bar{\bar{D}}_b\hat{S}_b$ expressed in the $|S,M_S\rangle$ coupled-spin basis, obtained with the spin-free NEVPT2 $J=-2.85$ cm^{-1} and the the calculated local anisotropy tensors shown in Eq. ?? of the main manuscript.

$\hat{H}^{MS}$	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3,3\|$	155.9	$0.6+0.4i$	$14.8-0.8i$	0	0	0	0	$39.4+35.3i$	$40.2+16.5i$	0	0	0	$18.2-0.9i$	0	0	0
$\langle 3,2\|$	$0.6-0.4i$	-6.4	$0.4+0.3i$	$21.0-1.1i$	0	0	0	-4.6	0	$40.2+16.5i$	0	0	$-0.4-0.2i$	$10.5-0.5i$	0	0
$\langle 3,1\|$	$14.8+0.8i$	$0.4-0.3i$	-103.8	$0.2+0.1i$	$23.0-1.2i$	0	0	$-30.5+27.4i$	-2.9	$-24.9-22.3i$	$31.2+12.7i$	0	79.5	$-0.3-0.2i$	$4.7-0.2i$	0
$\langle 3,0\|$	0	$21.0+1.1i$	$0.2-0.1i$	-136.3	$-0.2-0.1i$	$21.0-1.1i$	0	$-18.0+7.4i$	$-35.2+31.6i$	0	$-35.2-31.6i$	$18.0+7.4i$	$0.2-0.1i$	97.4	$-0.2-0.1i$	0
$\langle 3,-1\|$	0	0	$23.0+1.2i$	$-0.2+0.1i$	-103.8	$-0.4-0.3i$	$14.8-0.8i$	0	$-31.2+12.7i$	$-24.9+22.3i$	2.9	$-30.5-27.4i$	$4.7+0.2i$	$0.3-0.2i$	79.5	0
$\langle 3,-2\|$	0	0	0	$21.0+1.1i$	$-0.4+0.3i$	-6.4	$-0.6-0.4i$	0	0	$-40.2+16.5i$	0	4.6	0	$10.5+0.5i$	$0.4-0.2i$	0
$\langle 3,-3\|$	0	0	0	0	$14.8+0.8i$	$-0.6+0.4i$	155.9	0	0	0	$-40.2+16.5i$	$39.4-35.3i$	0	0	$18.2+0.9i$	0
$\langle 2,2\|$	$39.4-35.3i$	-4.6	$-30.5-27.4i$	$-18.0-7.4i$	0	0	0	2.1	0	0	0	0	$24.9+22.3i$	$36.0+14.7i$	0	$23.5-1.2i$
$\langle 2,1\|$	$40.2-16.5i$	0	-2.9	$-35.2-31.6i$	$-31.2-12.7i$	0	0	0	2.1	0	0	0	-3.6	$-17.6-15.8i$	$25.5+10.4i$	$-0.6-0.4i$
$\langle 2,0\|$	0	$40.2-16.5i$	$-24.9+22.3i$	0	$-24.9-22.3i$	$-40.2-16.5i$	0	0	0	2.1	0	0	$-30.5+27.4i$	0	$-30.5-27.4i$	162.3
$\langle 2,-1\|$	0	0	$31.2-12.7i$	$-35.2+31.6i$	2.9	0	$-40.2-16.5i$	0	0	0	2.1	0	$-25.5+10.4i$	$-17.6+15.8i$	3.6	$0.6-0.4i$
$\langle 2,-2\|$	0	0	0	$18.0-7.4i$	$-30.5+27.4i$	4.6	$39.4+35.3i$	0	0	0	0	2.1	0	$-36.0+14.7i$	$24.9-22.3i$	$23.5+1.2i$
$\langle 1,1\|$	$18.2+0.9i$	$-0.4+0.2i$	79.5	$0.2+0.1i$	$4.7-0.2i$	0	0	$24.9-22.3i$	-3.6	$-30.5-27.4i$	$-25.5-10.4i$	0	-57.1	$-0.4-0.3i$	$-23.0+1.2i$	0
$\langle 1,0\|$	0	$10.5+0.5i$	$-0.3+0.2i$	97.4	$0.3+0.2i$	$10.5-0.5i$	0	$36.0-14.7i$	$-17.6+15.8i$	0	$-17.6-15.8i$	$-36.0-14.7i$	$-0.4+0.3i$	137.7	$0.4+0.3i$	0
$\langle 1,-1\|$	0	0	$4.7+0.2i$	$-0.2+0.1i$	79.5	$0.4+0.2i$	$18.2-0.9i$	0	$25.5-10.4i$	$-30.5+27.4i$	3.6	$24.9+22.3i$	$-23.0-1.2i$	$0.4-0.3i$	-57.1	0
$\langle 0,0\|$	0	0	0	0	0	0	0	$23.5+1.2i$	$-0.6+0.4i$	162.3	$0.6+0.4i$	$23.5-1.2i$	0	0	0	10.7

Table S27 Complex 2: Matrix elements, in cm^{-1}, of $\hat{H}^{\text{eff}}$ expressed in the $|S,M_S\rangle$ coupled-spin basis, obtained from a SO-NEVPT2 calculation on complex 2 in the molecular PAF.

$\hat{H}^{\text{MS}}$	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3,3\|$	156.3	$0.2-0.3i$	$14.3+0.1i$	$0.2i$	0	0	0	$38.0+35.9i$	$39.9+15.7i$	0.1	$-0.1i$	0	$18.5-1.4i$	$-0.1i$	$-0.1i$	0.1
$\langle 3,2\|$	$0.2+0.3i$	-5.4	$0.1-0.1i$	$20.5-0.4i$	$0.1i$	0	0	$-5.9+0.3i$	0.4	$39.8+15.7i$	-0.1	0	$0.1i$	$10.5-0.6i$	0	0
$\langle 3,1\|$	$14.3-0.1i$	$0.1+0.1i$	-102.2	0	$22.5-0.5i$	$-0.1i$	0	$-30.2+27.6i$	$-3.6+0.1i$	$-24.8-22.7i$	$30.9+12.2i$	-0.1	79.3	$-0.1+0.1i$	$4.7-0.2i$	0.2
$\langle 3,0\|$	$-0.2i$	$20.5+0.4i$	0	-134.4	0	$20.5-0.4i$	$-0.2i$	$-17.9+7.1i$	$-34.9+32.0i$	$-0.1i$	$-34.9-32.0i$	$17.9+7.1i$	0.1	97.1	-0.1	0
$\langle 3,-1\|$	0	$-0.1i$	$22.5+0.5i$	0	-102.2	$-0.1+0.1i$	$14.3+0.1i$	-0.1	$-30.9+12.2i$	$-24.8+22.7i$	$3.6+0.1i$	$-30.2-27.6i$	$4.7+0.2i$	$0.1+0.1i$	79.3	-0.2
$\langle 3,-2\|$	0	0	$0.1i$	$20.5+0.4i$	$-0.1-0.1i$	-5.4	$-0.2+0.3i$	0	-0.1	$-39.9+15.7i$	0.4	$5.9+0.3i$	0	$10.5+0.6i$	$0.1i$	0
$\langle 3,-3\|$	0	0	0	$0.2i$	$14.3-0.1i$	$-0.2-0.3i$	156.3	0	$-0.1i$	0.1	$-39.9+15.7i$	$38.0-35.9i$	$0.1i$	$-0.1i$	$18.5+1.4i$	0.1
$\langle 2,2\|$	$38.0-35.9i$	$-5.9-0.3i$	$-30.2-27.6i$	$-17.9-7.1i$	-0.1	0	0	1.9	0.1	$0.2-0.3i$	$0.1i$	$0.1+0.1i$	$24.3+22.5i$	$35.8+14.1i$	0	$23.4-1.3i$
$\langle 2,1\|$	$39.9-15.7i$	0.4	$-3.6-0.1i$	$-34.9-32.0i$	$-30.9-12.2i$	-0.1	$0.1i$	0.1	2.2	$-0.2+0.1i$	$0.2-0.3i$	$-0.1i$	-4.1	$-17.5-16.1i$	$25.3+10.0i$	$-0.8+0.2i$
$\langle 2,0\|$	0.1	$39.8-15.7i$	$-24.8+22.7i$	$0.1i$	$-24.8-22.7i$	$-39.9-15.7i$	0.1	$0.2+0.3i$	$-0.2-0.1i$	2.3	$0.2-0.1i$	$0.2-0.3i$	$-30.3+27.8i$	0	$-30.3-27.8i$	161.5
$\langle 2,-1\|$	$0.1i$	-0.1	$30.9-12.2i$	$-34.9+32.0i$	$3.6-0.1i$	0.4	$-39.9-15.7i$	$-0.1i$	$0.2+0.3i$	$-0.2-0.1i$	2.2	-0.1	$-25.3+10.0i$	$-17.5+16.1i$	4.1	$0.8+0.2i$
$\langle 2,-2\|$	0	0	-0.1	$17.9-7.1i$	$-30.2+27.6i$	$5.9-0.3i$	$38.0+35.9i$	$0.1-0.1i$	$0.1i$	$-0.2-0.3i$	-0.1	1.9	0	$-35.8+14.1i$	$24.3-22.5i$	$23.4+1.3i$
$\langle 1,1\|$	$18.5+1.4i$	$-0.1i$	79.3	0.1	$4.7-0.2i$	0	$-0.1i$	$24.3-22.5i$	-4.1	$-30.3-27.8i$	$-25.3-10.0i$	0	-58.4	$-0.8+0.2i$	$-22.9+1.2i$	0.1
$\langle 1,0\|$	$0.1i$	$10.5+0.6i$	$-0.1-0.1i$	97.1	$0.1-0.1i$	$10.5-0.6i$	$0.1i$	$35.8-14.1i$	$-17.5+16.1i$	0	$-17.5-16.1i$	$-35.8-14.1i$	$-0.8-0.2i$	135.3	$0.8-0.2i$	0
$\langle 1,-1\|$	$0.1i$	0	$4.7+0.2i$	-0.1	79.3	$-0.1i$	$18.5-1.4i$	0	$25.3-10.0i$	$-30.3+27.8i$	4.1	$24.3+22.5i$	$-22.9-1.2i$	$0.8+0.2i$	-58.4	-0.1
$\langle 0,0\|$	0.1	0	0.2	0	0.2	0	0.1	$23.4+1.3i$	$-0.8-0.2i$	161.5	$0.8-0.2i$	$23.4-1.3i$	-0.1	0	-0.1	8.0

Table S28 Complex 2: Matrix elements, in cm^{-1}, of $\hat{H}^{\text{eff}}$ (Table S27) expressed in the uncoupled-spin basis, $|M_{Sa},M_{Sb}\rangle$.

$\hat{H}^{\text{MS}}$	$\|\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{1}{2}\rangle$	$\|\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{3}{2}\rangle$	$\|\frac{3}{2},-\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{1}{2},\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{3}{2}\rangle$	$\|\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{1}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},\frac{1}{2}\rangle$	$\|-\frac{1}{2},-\frac{3}{2}\rangle$	$\|-\frac{3}{2},-\frac{1}{2}\rangle$	$\|-\frac{3}{2},-\frac{3}{2}\rangle$
$\langle\frac{3}{2},\frac{3}{2}\|$	156.3	$27.0+25.2i$	$-26.7-25.6i$	$44.8+10.4i$	$-0.6+0.9i$	$-11.7-11.8i$	0.1	$0.1i$	$0.2i$	-0.1	$-0.1i$	0	0	0	0	0
$\langle\frac{3}{2},\frac{1}{2}\|$	$27.0-25.2i$	-7.6	$-3.6-0.3i$	0.1	$-27.4-25.3i$	-0.4	$44.8+10.2i$	$-0.2+0.2i$	$-11.9-11.6i$	$-0.1+0.2i$	$-0.1+0.1i$	0	0	0.1	0	0
$\langle\frac{1}{2},\frac{3}{2}\|$	$-26.7+25.6i$	$-3.6+0.3i$	4.1	0.3	$27.5+25.0i$	0	$-0.2+0.2i$	$44.5+10.7i$	$-0.1+0.3i$	$-11.7-12.1i$	0	0	$0.1+0.1i$	$-0.1i$	0.1	0
$\langle\frac{3}{2},-\frac{1}{2}\|$	$44.8-10.4i$	0.1	0.3	-3.5	$-4.1-0.1i$	-0.2	$-28.3-25.2i$	$-27.4-25.4i$	$0.1+0.1i$	0	0	$-11.8-11.8i$	$-0.1+0.3i$	$-0.1-0.1i$	0	0
$\langle\frac{1}{2},\frac{1}{2}\|$	$-0.6-0.9i$	$-27.4+25.3i$	$27.5-25.0i$	$-4.1+0.1i$	-162.4	$-3.8-0.1i$	0.3	-0.2	-0.1	0.3	$44.6+10.5i$	$-0.2+0.4i$	$-11.8-11.8i$	0	0	0
$\langle-\frac{1}{2},\frac{3}{2}\|$	$-11.7+11.8i$	-0.4	0	-0.2	$-3.8+0.1i$	7.4	0.1	$-0.2-0.1i$	$28.1+25.3i$	$27.0+25.5i$	$-0.2+0.2i$	$44.6+10.5i$	0	0	$0.1-0.1i$	$-0.1i$
$\langle\frac{3}{2},-\frac{3}{2}\|$	0.1	$44.8-10.2i$	$-0.2-0.2i$	$-28.4+25.2i$	0.4	0	166.6	-3.0	-0.2	0	$-27.0-25.5i$	-0.2	0	$-11.7-12.0i$	$0.2i$	0.1
$\langle\frac{1}{2},-\frac{1}{2}\|$	$-0.1i$	$-0.2-0.2i$	$44.5-10.7i$	$-27.3+25.4i$	$-0.3+0.1i$	-0.1	-3.0	-161.0	$-4.7+0.1i$	-0.2	$-28.0-25.2i$	0	0	$-0.1+0.3i$	$-11.9-11.6i$	$-0.2i$
$\langle-\frac{1}{2},\frac{1}{2}\|$	$-0.2i$	$-11.9+11.6i$	$-0.1-0.3i$	0	0	$28.0-25.2i$	-0.2	$-4.7-0.1i$	-161.0	-3.0	0.1	$0.3+0.1i$	$27.3+25.4i$	$44.5+10.7i$	$-0.2+0.2i$	$-0.1i$
$\langle-\frac{3}{2},\frac{3}{2}\|$	-0.1	$-0.2i$	$-11.7+12.0i$	0	0.2	$27.0-25.5i$	0	-0.2	-3.0	166.6	0	-0.4	$28.4+25.2i$	$-0.2+0.2i$	$44.8+10.2i$	-0.1
$\langle\frac{1}{2},-\frac{3}{2}\|$	$0.1i$	$-0.1-0.1i$	0	0	$44.6-10.5i$	$-0.2-0.2i$	$-27.2+25.5i$	$-28.1+25.2i$	0.2	0.2	7.4	$-3.8-0.1i$	-0.2	0	0.4	$-11.7-11.8i$
$\langle-\frac{1}{2},-\frac{1}{2}\|$	0	0	0	$-11.8+11.8i$	$-0.2-0.4i$	$44.6-10.5i$	-0.4	0.2	0.1	-0.2	$-3.8+0.1i$	-162.4	$-4.1-0.1i$	$-27.5-25.0i$	$27.4+25.3i$	$-0.6+0.9i$
$\langle-\frac{3}{2},\frac{1}{2}\|$	0	0	$0.1-0.1i$	$-0.1-0.3i$	$-11.8+11.8i$	0	$0.1i$	$0.2+0.1i$	$27.1-25.4i$	$28.3-25.2i$	-0.2	$-4.1+0.1i$	-3.5	-0.3	-0.1	$44.8+10.4i$
$\langle-\frac{1}{2},-\frac{3}{2}\|$	0	0.1	$0.1i$	$-0.1+0.1i$	0	0	$-11.8+11.8i$	$-0.2-0.5i$	$44.6-10.5i$	0	0	$-27.5+25.0i$	-0.3	4.1	$-3.6-0.3i$	$26.7+25.6i$
$\langle-\frac{3}{2},-\frac{1}{2}\|$	0	0	0.1	0	0	$0.1+0.1i$	0.1	$-11.8+11.8i$	$-0.3-0.4i$	$44.7-10.4i$	0.4	$27.4-25.3i$	-0.1	$-3.6+0.3i$	-7.6	$-27.0-25.2i$
$\langle-\frac{3}{2},-\frac{3}{2}\|$	0	0	0	0	0	$0.1i$	0.1	$0.2i$	$0.1i$	-0.1	$-11.7+11.8i$	$-0.6-0.9i$	$44.8-10.4i$	$26.7-25.6i$	$-27.0+25.2i$	156.3

Table S29 Complex 2: Matrix elements of $\hat{H}^{\mathrm{MS}} - \hat{H}^{\mathrm{eff}}$ (cm^{-1}) expressed in the $|M_{Sa}, M_{Sb}\rangle$ uncoupled-spin basis. $\hat{H}^{\mathrm{MS}} = J\hat{S}_a\hat{S}_b + \hat{S}_a\bar{\bar{D}}_a\hat{S}_a + \hat{S}_b\bar{\bar{D}}_b\hat{S}_b$ and $\hat{H}^{\mathrm{eff}}$ are taken from Tables S25 and S28 respectively.

Diff.	$\left\|\frac{3}{2},\frac{3}{2}\right\rangle$	$\left\|\frac{3}{2},\frac{1}{2}\right\rangle$	$\left\|\frac{1}{2},\frac{3}{2}\right\rangle$	$\left\|\frac{3}{2},-\frac{1}{2}\right\rangle$	$\left\|\frac{1}{2},\frac{1}{2}\right\rangle$	$\left\|-\frac{1}{2},\frac{3}{2}\right\rangle$	$\left\|\frac{3}{2},-\frac{3}{2}\right\rangle$	$\left\|\frac{1}{2},-\frac{1}{2}\right\rangle$	$\left\|-\frac{1}{2},\frac{1}{2}\right\rangle$	$\left\|-\frac{3}{2},\frac{3}{2}\right\rangle$	$\left\|\frac{1}{2},-\frac{3}{2}\right\rangle$	$\left\|-\frac{1}{2},-\frac{1}{2}\right\rangle$	$\left\|-\frac{3}{2},\frac{1}{2}\right\rangle$	$\left\|-\frac{1}{2},-\frac{3}{2}\right\rangle$	$\left\|-\frac{3}{2},-\frac{1}{2}\right\rangle$	$\left\|-\frac{3}{2},-\frac{3}{2}\right\rangle$
$\langle\frac{3}{2},\frac{3}{2}\|$	0.4	$-1.3-0.1i$	$0.8-0.9i$	$-0.3-0.4i$	$-0.6+0.9i$	$0.2+0.7i$	0.1	$0.1i$	$0.2i$	-0.1	$-0.1i$	0	0	0	0	0
$\langle\frac{3}{2},\frac{1}{2}\|$	$-1.3+0.1i$	-0.8	$0.6-0.3i$	0.1	$0.1-0.6i$	-0.4	$-0.3-0.6i$	$-0.2+0.2i$	$-0.1+0.9i$	$-0.1+0.2i$	$-0.1+0.1i$	0	0	0.1	0	0
$\langle\frac{1}{2},\frac{3}{2}\|$	$0.8+0.9i$	$0.6+0.3i$	1.6	0.3	$-0.8-0.2i$	0	$-0.2+0.2i$	$-0.5-0.1i$	$-0.1+0.3i$	$0.2+0.4i$	0	0	$0.1+0.1i$	$-0.1i$	0.1	0
$\langle\frac{3}{2},-\frac{1}{2}\|$	$-0.3+0.4i$	0.1	0.3	-1.0	$0.8-0.1i$	-0.2	$0.1i$	$0.1-0.7i$	$0.1+0.1i$	0	0	$0.6i$	$-0.1+0.3i$	$-0.1-0.1i$	0	0
$\langle\frac{1}{2},\frac{1}{2}\|$	$-0.6-0.9i$	$0.1+0.6i$	$-0.8+0.2i$	$0.8+0.1i$	0.7	$1.1-0.1i$	0.3	-0.2	-0.1	0.3	$-0.5-0.2i$	$-0.2+0.4i$	$0.6i$	0	0	0
$\langle-\frac{1}{2},\frac{3}{2}\|$	$0.2-0.7i$	-0.4	0	-0.2	$1.1+0.1i$	0.6	0.1	$-0.2-0.1i$	-0.2	$-0.5+0.8i$	$-0.2+0.2i$	$-0.5-0.2i$	0	0	$0.1-0.1i$	$-0.1i$
$\langle\frac{3}{2},-\frac{3}{2}\|$	0.1	$-0.3+0.6i$	$-0.2-0.2i$	$-0.1-0.1i$	0.4	0	-2.1	1.3	-0.2	0	$0.4-0.8i$	-0.2	0	$0.2+0.4i$	$0.2i$	0.1
$\langle\frac{1}{2},-\frac{1}{2}\|$	$-0.1i$	$-0.2-0.2i$	$-0.5+0.1i$	$0.1+0.7i$	$-0.3+0.1i$	-0.1	1.3	0.6	$1.0+0.1i$	-0.2	0.2	0	0	$-0.1+0.3i$	$-0.1+0.9i$	$-0.2i$
$\langle-\frac{1}{2},\frac{1}{2}\|$	$-0.2i$	$-0.1-0.9i$	$-0.1-0.3i$	0	0	-0.2	-0.2	$1.0-0.1i$	0.6	1.3	0.1	$0.3+0.1i$	$-0.1+0.7i$	$-0.5-0.1i$	$-0.2+0.2i$	$-0.1i$
$\langle-\frac{3}{2},\frac{3}{2}\|$	-0.1	$-0.2i$	$0.2-0.4i$	0	0.2	$-0.4-0.8i$	0	-0.2	1.3	-2.1	0	-0.4	$0.1-0.1i$	$-0.2+0.2i$	$-0.3-0.6i$	-0.1
$\langle\frac{1}{2},-\frac{3}{2}\|$	$0.1i$	$-0.1-0.1i$	0	0	$-0.5+0.2i$	$-0.2-0.2i$	$0.2+0.8i$	$0.2-0.1i$	0.2	0.2	0.6	$1.1-0.1i$	-0.2	0	0.4	$0.2+0.7i$
$\langle-\frac{1}{2},-\frac{1}{2}\|$	0	0	0	$-0.6i$	$-0.2-0.4i$	$-0.5+0.2i$	-0.4	0.2	0.1	-0.2	$1.1+0.1i$	0.7	$0.8-0.1i$	$0.8+0.2i$	$-0.1+0.6i$	$-0.6+0.9i$
$\langle-\frac{3}{2},\frac{1}{2}\|$	0	0	$0.1-0.1i$	$-0.1-0.3i$	$-0.6i$	0	$0.1i$	$0.2+0.1i$	$-0.4-0.7i$	0	-0.2	$0.8+0.1i$	-1.0	-0.3	-0.1	$-0.3-0.4i$
$\langle-\frac{1}{2},-\frac{3}{2}\|$	0	0.1	$0.1i$	$-0.1+0.1i$	0	0	$0.1-0.6i$	$-0.2-0.5i$	$-0.4+0.3i$	0	0	$0.8-0.2i$	-0.3	1.6	$0.6-0.3i$	$-0.8+0.9i$
$\langle-\frac{3}{2},-\frac{1}{2}\|$	0	0	0.1	0	0	$0.1+0.1i$	0.1	$-0.6i$	$-0.3-0.4i$	$-0.4+0.4i$	0.4	$-0.1-0.6i$	-0.1	$0.6+0.3i$	-0.8	$1.3+0.1i$
$\langle-\frac{3}{2},-\frac{3}{2}\|$	0	0	0	0	0	$0.1i$	0.1	$0.2i$	$0.1i$	-0.1	$0.2-0.7i$	$-0.6-0.9i$	$-0.3+0.4i$	$-0.8-0.9i$	$1.3-0.1i$	0.4

Table S30 Complex 2: Matrix elements of $\hat{H}^{\mathrm{MS}} - \hat{H}^{\mathrm{eff}}$ (cm^{-1}) expressed in the $|S, M_S\rangle$ coupled-spin basis. $\hat{H}^{\mathrm{MS}} = J\hat{S}_a\hat{S}_b + \hat{S}_a\bar{\bar{D}}_a\hat{S}_a + \hat{S}_b\bar{\bar{D}}_b\hat{S}_b$ and $\hat{H}^{\mathrm{eff}}$ are taken from Tables S26 and S27 respectively.

Diff.	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3,3\|$	0.4	$-0.4-0.6i$	$-0.5+0.8i$	$0.2i$	0	0	0	$-1.4+0.6i$	$-0.3-0.7i$	0.1	$-0.1i$	0	$0.3-0.4i$	$-0.1i$	$-0.1i$	0.1
$\langle 3,2\|$	$-0.4+0.6i$	1.1	$-0.4-0.4i$	$-0.5+0.7i$	$0.1i$	0	0	$-1.2+0.3i$	0.4	$-0.4-0.7i$	-0.1	0	$0.3+0.4i$	$-0.1i$	0	0
$\langle 3,1\|$	$-0.5-0.8i$	$-0.4+0.4i$	1.6	$-0.2-0.1i$	$-0.5+0.6i$	$-0.1i$	0	$0.3+0.2i$	$-0.7+0.1i$	$0.1-0.3i$	$-0.3-0.5i$	-0.1	-0.2	$0.2+0.3i$	0	0.2
$\langle 3,0\|$	$-0.2i$	$-0.5-0.7i$	$-0.2+0.1i$	1.9	$0.2+0.1i$	$-0.5+0.7i$	$-0.2i$	$0.1-0.2i$	$0.3+0.4i$	$-0.1i$	$0.3-0.4i$	$-0.1-0.2i$	$-0.1+0.1i$	-0.3	$0.1+0.1i$	0
$\langle 3,-1\|$	0	$-0.1i$	$-0.5-0.6i$	$0.2-0.1i$	1.6	$0.4+0.4i$	$-0.5+0.8i$	-0.1	$0.3-0.5i$	$0.1+0.3i$	$0.7+0.1i$	$0.3-0.2i$	0	$-0.2+0.3i$	-0.2	-0.2
$\langle 3,-2\|$	0	0	$0.1i$	$-0.5-0.7i$	$0.4-0.4i$	1.1	$0.4+0.6i$	0	-0.1	$0.4-0.7i$	0.4	$1.2+0.3i$	0	$0.1i$	$-0.3+0.4i$	0
$\langle 3,-3\|$	0	0	0	$0.2i$	$-0.5-0.8i$	$0.4-0.6i$	0.4	0	$-0.1i$	0.1	$0.3-0.7i$	$-1.4-0.6i$	$0.1i$	$-0.1i$	$0.3+0.4i$	0.1
$\langle 2,2\|$	$-1.4-0.6i$	$-1.2-0.3i$	$0.3-0.2i$	$0.1+0.2i$	-0.1	0	0	-0.2	0.1	$0.2-0.3i$	$0.1i$	$0.1+0.1i$	$-0.7+0.1i$	$-0.2-0.6i$	0	$-0.1-0.1i$
$\langle 2,1\|$	$-0.3+0.7i$	0.4	$-0.7-0.1i$	$0.3-0.4i$	$0.3+0.5i$	-0.1	$0.1i$	0.1	0.1	$-0.2+0.1i$	$0.2-0.3i$	$-0.1i$	-0.5	$0.1-0.3i$	$-0.2-0.4i$	$-0.2+0.5i$
$\langle 2,0\|$	0.1	$-0.4+0.7i$	$0.1+0.3i$	$0.1i$	$0.1-0.3i$	$0.4+0.7i$	0.1	$0.2+0.3i$	$-0.2-0.1i$	0.2	$0.2-0.1i$	$0.2-0.3i$	$0.2+0.4i$	0	$0.2-0.4i$	-0.9
$\langle 2,-1\|$	$0.1i$	-0.1	$-0.3+0.5i$	$0.3+0.4i$	$0.7-0.1i$	0.4	$0.3+0.7i$	$-0.1i$	$0.2+0.3i$	$-0.2-0.1i$	0.1	-0.1	$0.2-0.4i$	$0.1+0.3i$	0.5	$0.2+0.5i$
$\langle 2,-2\|$	0	0	-0.1	$-0.1+0.2i$	$0.3+0.2i$	$1.2-0.3i$	$-1.4+0.6i$	$0.1-0.1i$	$0.1i$	$-0.2-0.3i$	-0.1	-0.2	0	$0.2-0.6i$	$-0.7-0.1i$	$-0.1+0.1i$
$\langle 1,1\|$	$0.3+0.4i$	$0.3-0.4i$	-0.2	$-0.1-0.1i$	0	0	$-0.1i$	$-0.7-0.1i$	-0.5	$0.2-0.4i$	$0.2+0.4i$	0	-1.3	$-0.4+0.4i$	0.1	0.1
$\langle 1,0\|$	$0.1i$	$0.1i$	$0.2-0.3i$	-0.3	$-0.2-0.3i$	$-0.1i$	$0.1i$	$-0.2+0.6i$	$0.1+0.3i$	0	$0.1-0.3i$	$0.2+0.6i$	$-0.4-0.4i$	-2.4	$0.4-0.4i$	0
$\langle 1,-1\|$	$0.1i$	0	0	$0.1-0.1i$	-0.2	$-0.3-0.4i$	$0.3-0.4i$	0	$-0.2+0.4i$	$0.2+0.4i$	0.5	$-0.7+0.1i$	0.1	$0.4+0.4i$	-1.3	-0.1
$\langle 0,0\|$	0.1	0	0.2	0	0.2	0	0.1	$-0.1+0.1i$	$-0.2-0.5i$	-0.9	$0.2-0.5i$	$-0.1-0.1i$	-0.1	0	-0.1	-2.7

Table S31 Analytical matrix elements of $\hat{S}_a\bar{\bar{D}}_{ab}\hat{S}_b$ for dicobalt(II) complexes expressed, in the molecular PAF, in the $|S,M_S\rangle$ coupled spin-basis spanned by the $S=3,2,1,0$ spin functions.

$\hat{S}_a\bar{\bar{D}}_{ab}\hat{S}_b$	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3,3\|$	$\frac{3D_{ab}}{2}$	0	$\frac{3\sqrt{15}E_{ab}}{10}$	0	0	0	0	0	0	0	0	0	$-\frac{3\sqrt{10}E_{ab}}{10}$	0	0	0
$\langle 3,2\|$	0	0	0	$\frac{3\sqrt{30}E_{ab}}{10}$	0	0	0	0	0	0	0	0	0	$-\frac{\sqrt{30}E_{ab}}{10}$	0	0
$\langle 3,1\|$	$\frac{3\sqrt{15}E_{ab}}{10}$	0	$-\frac{9D_{ab}}{10}$	0	$\frac{9E_{ab}}{5}$	0	0	0	0	0	0	0	$-\frac{\sqrt{6}D_{ab}}{5}$	0	$-\frac{\sqrt{6}E_{ab}}{10}$	0
$\langle 3,0\|$	0	$\frac{3\sqrt{30}E_{ab}}{10}$	0	$-\frac{3D_{ab}}{5}+\frac{9E_{ab}}{5}$	0	$\frac{3\sqrt{30}E_{ab}}{10}$	0	0	0	0	0	0	0	$-\frac{4D_{ab}}{5}-\frac{3E_{ab}}{5}$	0	0
$\langle 3,-1\|$	0	0	$\frac{9E_{ab}}{5}$	0	$-\frac{9D_{ab}}{10}$	0	$\frac{3\sqrt{15}E_{ab}}{10}$	0	0	0	0	0	$-\frac{\sqrt{6}E_{ab}}{10}$	0	$-\frac{\sqrt{6}D_{ab}}{5}$	0
$\langle 3,-2\|$	0	0	0	$\frac{3\sqrt{30}E_{ab}}{10}$	0	0	0	0	0	0	0	0	0	$-\frac{\sqrt{30}E_{ab}}{10}$	0	0
$\langle 3,-3\|$	0	0	0	0	$\frac{3\sqrt{15}E_{ab}}{10}$	0	$\frac{3D_{ab}}{2}$	0	0	0	0	0	0	0	$-\frac{3\sqrt{10}E_{ab}}{10}$	0
$\langle 2,2\|$	0	0	0	0	0	0	0	D_{ab}	0	$\frac{\sqrt{6}E_{ab}}{2}$	0	0	0	0	0	$-\frac{\sqrt{6}E_{ab}}{2}$
$\langle 2,1\|$	0	0	0	0	0	0	0	0	$-\frac{D_{ab}}{2}$	0	$\frac{3E_{ab}}{2}$	0	0	0	0	0
$\langle 2,0\|$	0	0	0	0	0	0	0	$\frac{\sqrt{6}E_{ab}}{2}$	0	$-\frac{4D_{ab}}{3}-E_{ab}$	0	$\frac{\sqrt{6}E_{ab}}{2}$	0	0	0	$-\frac{2D_{ab}}{3}+E_{ab}$
$\langle 2,-1\|$	0	0	0	0	0	0	0	0	$\frac{3E_{ab}}{2}$	0	$-\frac{D_{ab}}{2}$	0	0	0	0	0
$\langle 2,-2\|$	0	0	0	0	0	0	0	0	0	$\frac{\sqrt{6}E_{ab}}{2}$	0	D_{ab}	0	0	0	$-\frac{\sqrt{6}E_{ab}}{2}$
$\langle 1,1\|$	$-\frac{3\sqrt{10}E_{ab}}{10}$	0	$-\frac{\sqrt{6}D_{ab}}{5}$	0	$-\frac{\sqrt{6}E_{ab}}{10}$	0	0	0	0	0	0	0	$\frac{17D_{ab}}{30}$	0	$\frac{17E_{ab}}{10}$	0
$\langle 1,0\|$	0	$-\frac{\sqrt{30}E_{ab}}{10}$	0	$-\frac{4D_{ab}}{5}-\frac{3E_{ab}}{5}$	0	$-\frac{\sqrt{30}E_{ab}}{10}$	0	0	0	0	0	0	0	$-\frac{16D_{ab}}{15}+\frac{E_{ab}}{5}$	0	0
$\langle 1,-1\|$	0	0	$-\frac{\sqrt{6}E_{ab}}{10}$	0	$-\frac{\sqrt{6}D_{ab}}{5}$	0	$-\frac{3\sqrt{10}E_{ab}}{10}$	0	0	0	0	0	$\frac{17E_{ab}}{10}$	0	$\frac{17D_{ab}}{30}$	0
$\langle 0,0\|$	0	0	0	0	0	0	0	$-\frac{\sqrt{6}E_{ab}}{2}$	0	$-\frac{2D_{ab}}{3}+E_{ab}$	0	$-\frac{\sqrt{6}E_{ab}}{2}$	0	0	0	$-\frac{D_{ab}}{3}-E_{ab}$

Table S32 Complex 2: Numerical matrix elements (cm^{-1}) of $\hat{H}^{MS} = J\hat{S}_a\hat{S}_b + \left[\hat{S}_a\bar{\bar{D}}_a\hat{S}_a + \hat{S}_b\bar{\bar{D}}_b\hat{S}_b\right]_{calc} + \hat{S}_a\bar{\bar{D}}_{ab}\hat{S}_b$, expressed in the $|S,M_S\rangle$ coupled-spin basis, obtained with calculated local anisotropies and J, D_{ab}, E_{ab} listed in Equation ?? and Table ??, respectively, of the main manuscript.

$\hat{H}^{MS}$	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3,3\|$	157.1	$0.6+0.4i$	$14.7-0.8i$	0	0	0	0	$39.4+35.3i$	$40.2+16.5i$	0	0	0	$18.3-0.9i$	0	0	0
$\langle 3,2\|$	$0.6-0.4i$	-5.1	$0.4+0.3i$	$20.8-1.1i$	0	0	0	-4.6	0	$40.2+16.5i$	0	0	$-0.4-0.2i$	$10.6-0.5i$	0	0
$\langle 3,1\|$	$14.7+0.8i$	$0.4-0.3i$	-102.4	$0.2+0.1i$	$22.8-1.2i$	0	0	$-30.5+27.4i$	-2.9	$-24.9-22.3i$	$31.2+12.7i$	0	79.6	$-0.3-0.2i$	$4.7-0.2i$	0
$\langle 3,0\|$	0	$20.8+1.1i$	$0.2-0.1i$	-135.2	$-0.2-0.1i$	$20.8-1.1i$	0	$-18.0+7.4i$	$-35.2+31.6i$	0	$-35.2-31.6i$	$18.0+7.4i$	$0.2-0.1i$	97.5	$-0.2-0.1i$	0
$\langle 3,-1\|$	0	0	$22.8+1.2i$	$-0.2+0.1i$	-102.4	$-0.4-0.3i$	$14.7-0.8i$	0	$-31.2+12.7i$	$-24.9+22.3i$	2.9	$-30.5-27.4i$	$4.7+0.2i$	$0.3-0.2i$	79.6	0
$\langle 3,-2\|$	0	0	0	$20.8+1.1i$	$-0.4+0.3i$	-5.1	$-0.6-0.4i$	0	0	$-40.2+16.5i$	0	4.6	0	$10.6+0.5i$	$0.4-0.2i$	0
$\langle 3,-3\|$	0	0	0	0	$14.7+0.8i$	$-0.6+0.4i$	157.1	0	0	0	$-40.2+16.5i$	$39.4-35.3i$	0	0	$18.3+0.9i$	0
$\langle 2,2\|$	$39.4-35.3i$	-4.6	$-30.5-27.4i$	$-18.0-7.4i$	0	0	0	1.6	0	-0.2	0	0	$24.9+22.3i$	$36.0+14.7i$	0	$23.6-1.2i$
$\langle 2,1\|$	$40.2-16.5i$	0	-2.9	$-35.2-31.6i$	$-31.2-12.7i$	0	0	0	1.7	0	-0.2	0	-3.6	$-17.6-15.8i$	$25.5+10.4i$	$-0.6-0.4i$
$\langle 2,0\|$	0	$40.2-16.5i$	$-24.9+22.3i$	0	$-24.9-22.3i$	$-40.2-16.5i$	0	-0.2	0	1.9	0	-0.2	$-30.5+27.4i$	0	$-30.5-27.4i$	162.2
$\langle 2,-1\|$	0	0	$31.2-12.7i$	$-35.2+31.6i$	2.9	0	$-40.2-16.5i$	0	-0.2	0	1.7	0	$-25.5+10.4i$	$-17.6+15.8i$	3.6	$0.6-0.4i$
$\langle 2,-2\|$	0	0	0	$18.0-7.4i$	$-30.5+27.4i$	4.6	$39.4+35.3i$	0	0	-0.2	0	1.6	0	$-36.0+14.7i$	$24.9-22.3i$	$23.6+1.2i$
$\langle 1,1\|$	$18.3+0.9i$	$-0.4+0.2i$	79.6	$0.2+0.1i$	$4.7-0.2i$	0	0	$24.9-22.3i$	-3.6	$-30.5-27.4i$	$-25.5-10.4i$	0	-58.7	$-0.4-0.3i$	$-23.2+1.2i$	0
$\langle 1,0\|$	0	$10.6+0.5i$	$-0.3+0.2i$	97.5	$0.3+0.2i$	$10.6-0.5i$	0	$36.0-14.7i$	$-17.6+15.8i$	0	$-17.6-15.8i$	$-36.0-14.7i$	$-0.4+0.3i$	136.2	$0.4+0.3i$	0
$\langle 1,-1\|$	0	0	$4.7+0.2i$	$-0.2+0.1i$	79.6	$0.4+0.2i$	$18.3-0.9i$	0	$25.5-10.4i$	$-30.5+27.4i$	3.6	$24.9+22.3i$	$-23.2-1.2i$	$0.4-0.3i$	-58.7	0
$\langle 0,0\|$	0	0	0	0	0	0	0	$23.6+1.2i$	$-0.6+0.4i$	162.2	$0.6+0.4i$	$23.6-1.2i$	0	0	0	8.7

Table S33 Complex 2: Matrix elements of $\hat{H}^{MS} - \hat{H}^{eff}$ (cm^{-1}) expressed in the $|S,M_S\rangle$ coupled-spin basis. $\hat{H}^{MS}$ and $\hat{H}^{eff}$ matrices are taken from Tables S32 and S27 respectively.

Diff.	$\|3,3\rangle$	$\|3,2\rangle$	$\|3,1\rangle$	$\|3,0\rangle$	$\|3,-1\rangle$	$\|3,-2\rangle$	$\|3,-3\rangle$	$\|2,2\rangle$	$\|2,1\rangle$	$\|2,0\rangle$	$\|2,-1\rangle$	$\|2,-2\rangle$	$\|1,1\rangle$	$\|1,0\rangle$	$\|1,-1\rangle$	$\|0,0\rangle$
$\langle 3,3\|$	0.8	$0.4+0.6i$	$0.4-0.8i$	$-0.2i$	0	0	0	$1.4-0.6i$	$0.3+0.7i$	-0.1	$0.1i$	0	$-0.2+0.4i$	$0.1i$	$0.1i$	-0.1
$\langle 3,2\|$	$0.4-0.6i$	0.2	$0.4+0.4i$	$0.3-0.7i$	$-0.1i$	0	0	$1.2-0.3i$	-0.4	$0.4+0.7i$	0.1	0	$-0.3-0.4i$	$0.1+0.1i$	0	0
$\langle 3,1\|$	$0.4+0.8i$	$0.4-0.4i$	-0.2	$0.2+0.1i$	$0.2-0.6i$	$0.1i$	0	$-0.3-0.2i$	$0.7-0.1i$	$-0.1+0.3i$	$0.3+0.5i$	0.1	0.3	$-0.2-0.3i$	0.1	-0.2
$\langle 3,0\|$	$0.2i$	$0.3+0.7i$	$0.2-0.1i$	-0.7	$-0.2-0.1i$	$0.3-0.7i$	$0.2i$	$-0.1+0.2i$	$-0.3-0.4i$	$0.1i$	$-0.3+0.4i$	$0.1+0.2i$	$0.1-0.1i$	0.4	$-0.1-0.1i$	0
$\langle 3,-1\|$	0	$0.1i$	$0.2+0.6i$	$-0.2+0.1i$	-0.2	$-0.4-0.4i$	$0.4-0.8i$	0.1	$-0.3+0.5i$	$-0.1-0.3i$	$-0.7-0.1i$	$-0.3+0.2i$	0.1	$0.2-0.3i$	0.3	0.2
$\langle 3,-2\|$	0	0	$-0.1i$	$0.3+0.7i$	$-0.4+0.4i$	0.2	$-0.4-0.6i$	0	0.1	$-0.4+0.7i$	-0.4	$-1.2-0.3i$	0	$0.1-0.1i$	$0.3-0.4i$	0
$\langle 3,-3\|$	0	0	0	$-0.2i$	$0.4+0.8i$	$-0.4+0.6i$	0.8	0	$0.1i$	-0.1	$-0.3+0.7i$	$1.4+0.6i$	$-0.1i$	$0.1i$	$-0.2-0.4i$	-0.1
$\langle 2,2\|$	$1.4+0.6i$	$1.2+0.3i$	$-0.3+0.2i$	$-0.1-0.2i$	0.1	0	0	-0.3	-0.1	$-0.3+0.3i$	$-0.1i$	$-0.1-0.1i$	$0.7-0.1i$	$0.2+0.6i$	0	$0.2+0.1i$
$\langle 2,1\|$	$0.3-0.7i$	-0.4	$0.7+0.1i$	$-0.3+0.4i$	$-0.3-0.5i$	0.1	$-0.1i$	-0.1	-0.5	$0.2-0.1i$	$-0.3+0.3i$	$0.1i$	0.5	$-0.1+0.3i$	$0.2+0.4i$	$0.2-0.5i$
$\langle 2,0\|$	-0.1	$0.4-0.7i$	$-0.1-0.3i$	$-0.1i$	$-0.1+0.3i$	$-0.4-0.7i$	-0.1	$-0.3-0.3i$	$0.2+0.1i$	-0.4	$-0.2+0.1i$	$-0.3+0.3i$	$-0.2-0.4i$	0	$-0.2+0.4i$	0.8
$\langle 2,-1\|$	$-0.1i$	0.1	$0.3-0.5i$	$-0.3-0.4i$	$-0.7+0.1i$	-0.4	$-0.3-0.7i$	$0.1i$	$-0.3-0.3i$	$0.2+0.1i$	-0.5	0.1	$-0.2+0.4i$	$-0.1-0.3i$	-0.5	$-0.2-0.5i$
$\langle 2,-2\|$	0	0	0.1	$0.1-0.2i$	$-0.3-0.2i$	$-1.2+0.3i$	$1.4-0.6i$	$-0.1+0.1i$	$-0.1i$	$0.3i$	0.1	-0.3	0	$-0.2+0.6i$	$0.7+0.1i$	$0.2-0.1i$
$\langle 1,1\|$	$-0.2-0.4i$	$-0.3+0.4i$	0.3	$0.1+0.1i$	0.1	0	$0.1i$	$0.7+0.1i$	0.5	$-0.2+0.4i$	$-0.2-0.4i$	0	-0.3	$0.4-0.4i$	-0.4	-0.1
$\langle 1,0\|$	$-0.1i$	$0.1-0.1i$	$-0.2+0.3i$	0.4	$0.2+0.3i$	$0.1+0.1i$	$-0.1i$	$0.2-0.6i$	$-0.1-0.3i$	0	$-0.1+0.3i$	$-0.2-0.6i$	$0.4+0.4i$	0.9	$-0.4+0.4i$	0
$\langle 1,-1\|$	$-0.1i$	0	0.1	$-0.1+0.1i$	0.3	$0.3+0.4i$	$-0.2+0.4i$	0	$0.2-0.4i$	$-0.2-0.4i$	-0.5	$0.7-0.1i$	-0.4	$-0.4-0.4i$	-0.3	0.1
$\langle 0,0\|$	-0.1	0	-0.2	0	-0.2	0	-0.1	$0.2-0.1i$	$0.2+0.5i$	0.8	$-0.2+0.5i$	$0.2+0.1i$	0.1	0	0.1	0.7

S2 xyz coordinates

S2.1 Complex 1: $[Co_2Cl_6]^{2-}$

Arbitrary frame:

Co	-0.000682	0.004123	-1.595481
Co	0.000682	-0.004123	1.595481
Cl	0.000000	-1.717325	0.000000
Cl	1.895916	-0.178834	-2.743890
Cl	-1.861051	0.153232	-2.805935
Cl	0.000000	1.717325	-0.000000
Cl	-1.895916	0.178834	2.743890
Cl	1.861051	-0.153232	2.805935

Molecular PAF:

Co	-1.587716	-0.136461	0.078181
Co	1.587716	0.136461	-0.078181
Cl	-0.048059	-0.351600	-1.680260
Cl	-2.557145	-2.122392	0.334479
Cl	-2.963284	1.603233	-0.094113
Cl	0.048059	0.351600	1.680260
Cl	2.557145	2.122392	-0.334479
Cl	2.963284	-1.603233	0.094113

S2.2 Complex 2: $[Co_2(L)_2(acac)_2(H_2O)]$

Arbitrary frame:

O	0.113492	-1.374674	-0.077237
Co	0.016448	0.115158	-1.554198
Co	-0.018680	-0.109455	1.565701
O	-0.319718	1.222363	3.089591
O	0.000432	1.389143	0.007798
O	-2.112259	-0.119467	1.251910
H	-2.566740	-0.907787	1.597783
H	-2.243365	-0.141475	0.253473
O	1.975431	0.158534	1.798366
O	-2.030940	-0.098165	-1.451936
O	-0.237416	1.408603	-3.105331
O	0.092614	-1.469756	-2.913571
N	-0.059152	-1.808842	2.759532
N	2.083351	0.416352	-1.629002
C	0.564069	1.931802	3.678787
C	-0.770256	-3.319332	0.982473
C	-0.434915	-2.952446	2.355083
H	-0.503954	-3.793547	3.070450
C	0.701539	2.498988	0.027175
C	1.966996	2.602957	-0.618920
C	0.220071	3.632736	0.700156
C	-0.449995	-2.550761	-0.158652
C	-0.735973	-3.153432	-1.414724
C	-1.375494	-4.565359	0.853066
H	-1.588155	-5.130032	1.772610
C	-2.860978	0.246368	-2.355766
C	2.551072	1.010673	2.523319
C	1.923858	1.844741	3.440702
H	2.571187	2.521007	4.010060
C	-1.099940	3.609857	1.317907

H	-1.663625	2.652511	1.197804
C	-1.708827	-5.126159	-0.377668
C	-2.546186	0.999344	-3.445803
C	2.595889	1.523487	-1.299456
H	3.663564	1.712413	-1.547700
C	-1.344872	-4.411890	-1.486602
H	-1.533774	-4.828295	-2.487513
C	-0.376233	-2.582105	-2.676728
H	-0.562981	-3.254792	-3.552925
H	-1.449124	-2.652236	5.980214
C	-0.539125	-3.258345	5.878647
C	0.318757	-1.638219	4.180843
H	-0.416620	-0.936334	4.617335
H	1.277453	-1.085958	4.164811
C	-0.423979	-4.417566	6.623957
C	0.050577	2.904875	4.691326
H	-0.581399	3.661968	4.189807
H	0.856567	3.420210	5.238207
H	-0.602258	2.383176	5.414714
C	0.448015	-2.875103	5.013415
C	3.682513	-1.741578	-0.110669
H	2.622296	-1.899261	0.113777
C	-4.277203	-0.224867	-2.160618
H	-4.296355	-1.327852	-2.081622
H	-4.949842	0.085316	-2.976063
H	-4.676485	0.171190	-1.207669
C	4.045327	1.105327	2.340558
H	4.532029	0.213702	2.772093
H	4.474943	2.004226	2.812365
H	4.283448	1.109595	1.262796
C	-2.371102	-6.465188	-0.459840
H	-1.812382	-7.232655	0.107574
H	-2.452770	-6.816577	-1.502735
H	-3.394815	-6.441024	-0.039746
C	1.565054	-3.674520	4.932264
H	2.384000	-3.391249	4.262072
C	3.016039	-0.576199	-2.242488
H	3.506234	-0.118504	-3.124101
H	2.401409	-1.411023	-2.617514
C	4.049676	-1.063389	-1.274319
C	4.655030	-2.200927	0.768833
C	0.692801	-5.209407	6.516260
H	0.761142	-6.132143	7.106360
F	-1.726798	-6.112369	7.557215
C	-1.502240	-4.816766	7.563022
F	-2.660718	-4.242148	7.305607
F	-1.239495	-4.511708	8.808129
C	4.279066	-2.887951	2.004205
F	3.056259	-3.437514	1.948283
F	4.244695	-2.079687	3.052563
F	5.088540	-3.868775	2.352848
C	1.682326	-4.836019	5.697083
H	2.592398	-5.442117	5.601930
C	5.401009	-0.853778	-1.529788
H	5.703744	-0.326985	-2.444567
C	6.001439	-1.977793	0.491513

H	6.773111	-2.346500	1.177712
C	6.342486	-1.293225	-0.645868
H	7.405444	-1.116734	-0.859792
O	-1.596394	4.553136	1.898839
C	2.673551	3.798467	-0.529406
H	3.658107	3.843182	-1.020668
C	-1.296880	1.537853	-3.760791
C	0.983257	4.809942	0.748140
H	0.541497	5.657760	1.291951
H	-3.357897	1.220261	-4.147388
C	2.211621	4.914082	0.137340
C	3.008678	6.200682	0.185976
H	3.094622	6.583589	1.219155
H	2.525519	6.995864	-0.413030
H	4.030009	6.062093	-0.209204
C	-1.164294	2.360590	-5.013161
H	-0.769726	3.360285	-4.755399
H	-2.110876	2.482281	-5.564556
H	-0.419100	1.889569	-5.680001

Molecular PAF:

O	-0.195445	0.946496	-0.987178
Co	1.328819	0.688948	0.434342
Co	-1.338206	-0.697582	-0.431663
O	-2.451548	-2.243338	0.315139
O	0.313972	-0.979562	0.933627
O	-2.133707	0.526377	1.101550
H	-2.832311	1.136828	0.806708
H	-1.373539	1.108085	1.415093
O	-0.465787	-2.011719	-1.702237
O	0.163317	1.823982	1.699673
O	2.790580	0.685822	1.850925
O	2.133582	2.443892	-0.364518
N	-2.744314	-0.081519	-1.830989
N	2.501547	-0.531414	-0.791965
C	-2.333421	-3.483884	0.034736
C	-1.971153	2.228824	-1.929614
C	-2.860477	1.114221	-2.242473
H	-3.684750	1.381620	-2.930252
C	0.906817	-2.123501	1.185861
C	2.106065	-2.513634	0.523118
C	0.365383	-3.012813	2.127175
C	-0.682595	2.098343	-1.365674
C	0.080207	3.295176	-1.273820
C	-2.455499	3.474945	-2.314625
H	-3.458374	3.518720	-2.764031
C	0.577196	2.454761	2.726999
C	-0.582990	-3.264445	-1.702965
C	-1.470399	-3.991909	-0.919410
H	-1.462497	-5.079529	-1.051927
C	-0.819049	-2.637812	2.889450
H	-1.223661	-1.620092	2.667612
C	-1.727990	4.653663	-2.167418
C	1.816869	2.312421	3.272156
C	2.740553	-1.733283	-0.483047
H	3.528532	-2.282141	-1.044378

C	-0.456745	4.523076	-1.678274
H	0.185450	5.412222	-1.589365
C	1.443818	3.343732	-0.841745
H	1.924183	4.349305	-0.956536
H	-6.320278	-0.398151	-2.189255
C	-5.917117	-0.382362	-3.210526
C	-3.697991	-1.104240	-2.317397
H	-4.269973	-1.443366	-1.433215
H	-3.074473	-1.969321	-2.612706
C	-6.746892	0.000185	-4.248635
C	-3.210732	-4.414167	0.809771
H	-2.936942	-4.374771	1.881029
H	-3.141305	-5.457847	0.463101
H	-4.262083	-4.079531	0.743937
C	-4.611215	-0.717992	-3.438379
C	1.545371	-0.585860	-3.724895
H	0.788164	-0.050801	-3.142100
C	-0.407209	3.404881	3.354738
H	-0.736903	4.149528	2.606415
H	0.004439	3.935849	4.227794
H	-1.310407	2.851791	3.675242
C	0.343587	-3.995838	-2.641943
H	0.023881	-3.832187	-3.685544
H	0.374380	-5.080734	-2.448961
H	1.361820	-3.579777	-2.550378
C	-2.301830	5.970314	-2.586343
H	-2.669770	5.942295	-3.628920
H	-1.555681	6.780541	-2.518757
H	-3.161620	6.261248	-1.952964
C	-4.165339	-0.681495	-4.739645
H	-3.129581	-0.959433	-4.963315
C	3.253258	0.000545	-1.968137
H	4.339673	-0.127597	-1.794070
H	3.063475	1.085653	-2.011370
C	2.855469	-0.665341	-3.249335
C	1.197038	-1.195963	-4.923541
C	-6.277299	0.044784	-5.538326
H	-6.946905	0.362677	-6.347586
F	-8.570788	1.382523	-4.699427
C	-8.163839	0.356182	-3.985239
F	-8.400528	0.668024	-2.726170
F	-8.997824	-0.614419	-4.258713
C	-0.179243	-1.141732	-5.415886
F	-0.875254	-0.108821	-4.916820
F	-0.883058	-2.216764	-5.095767
F	-0.287932	-1.037340	-6.725888
C	-5.010811	-0.308192	-5.785400
H	-4.612951	-0.295659	-6.808234
C	3.797098	-1.368702	-3.993593
H	4.832640	-1.433861	-3.633890
C	2.157498	-1.895386	-5.650065
H	1.889844	-2.370683	-6.601246
C	3.434042	-1.979278	-5.158151
H	4.188204	-2.534199	-5.732688
O	-1.335302	-3.339707	3.734761
C	2.663008	-3.755599	0.812625

H	3.578208	-4.039446	0.269921
C	2.832489	1.459560	2.834983
C	0.981206	-4.249800	2.374549
H	0.501399	-4.893766	3.126061
H	2.043097	2.919466	4.155456
C	2.132426	-4.638948	1.729525
C	2.789984	-5.970223	2.026724
H	2.061345	-6.799882	1.979678
H	3.228673	-5.984099	3.042561
H	3.601453	-6.192078	1.312028
C	4.131630	1.441748	3.593153
H	4.346216	0.410981	3.929289
H	4.142009	2.111548	4.468437
H	4.953560	1.729122	2.912199