Electronic Supplementary Information (ESI)

Non-Empirical Calculation of X-ray Magnetic Circular Dichroism in Lanthanide Compounds

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Computational Details

The DFT calculations were performed by means of the Amsterdam density functional (ADF) program package.[1] The main results reported in this work are obtained using the local density approximation (LDA) following the Slater exchange and Vosko-Wilk-Nusair correlation (SVWN) formulation[2] as well as the generalized gradient approximation (GGA) functional following the Perdew-Burke-Erzerhof (PBE) parameterization.[3] The test of the influence of the DFT functional, including various LDA and other GGA reveals *a priori* a minor variation in the theoretical results. The molecular orbitals were expanded using multiple-zeta Slater-type orbital (STO) functions with polarization extra functions,[4] *i.e.*, TZ2P for the terbium atom and TZP for nitrogen, carbon and hydrogen atoms.

The DFT calculations were done using the average of configuration (AOC) method, which allows one to obtain a statistically averaged electron density in Slater's sense that is well suited to resolve the ligand-field states. The AOC method forces fractional occupation of electrons within Kohn-Sham orbitals that are selectively chosen as the active subspace. This active subspace forms the basis of the terbium $3d$ and $4f$ orbitals. The ligand-field concept is useful, as long as these active orbitals are not excessively delocalized in the Kohn-Sham molecular orbital schemes obtained for TbPc$_2$. The self-consistent field was set up to take into account all electrons. The relativistic corrections are treated with the Zeroth-Order Regular Approximation (ZORA) of the Dirac equation method.[5] All electronic structure calculations were done at the scalar ZORA relativistic level of theory, and spin-orbit coupling interaction was included through the use of the spin-orbit ZORA method.[5] The non-empirical parameters that input the effective ligand-field Hamiltonian in Eq. 1 were obtained using the newly available LFDFT keyword in the ADF program package.[1]

To optimize the TbPc$_2$ geometry, the following points have been adopted: (1) the molecular complex was assumed to be of D_{4d} conformation, which point group was available in the ADF program package;[1] (2) eight electrons were evenly distributed over the sevenfold Kohn-Sham orbitals that have predominant Tb $4f$ character.

References
1   E. J. Baerends *et al.*, ADF2017, 2017, available at http://www.scm.com.
2   S. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.*, 1980, **58**, 1200–1211.
3   J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865–3868.
4   E. V. Lenthe and E. J. Baerends, *J. Comput. Chem.*, 2003, **24**, 1142–1156.
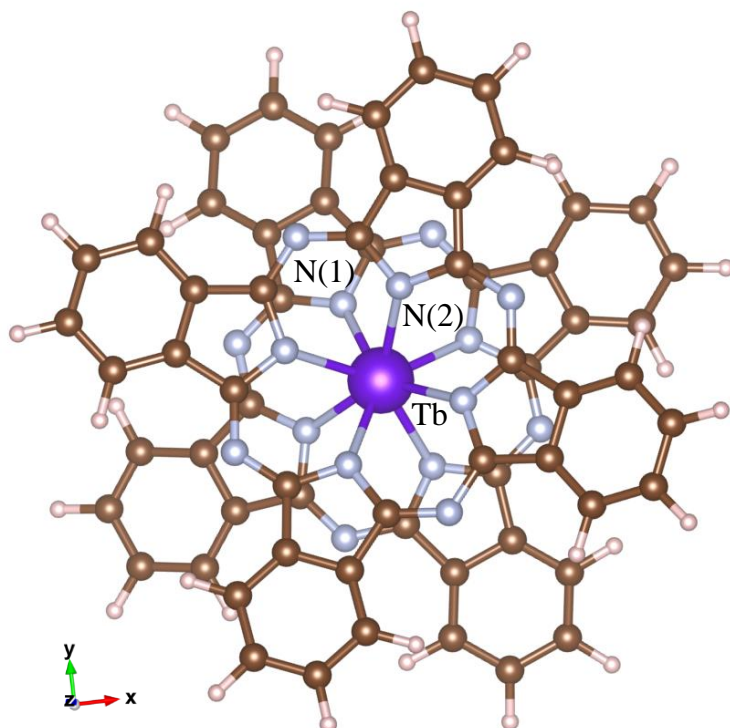5   E. van Lenthe, E. J. Baerends and J. G. Snijders, *J. Chem. Phys.*, 1993, **99**, 4597–4610.

Figure S1. Graphical representation of the optimized molecular structure of the TbPc$_2$ complex with D_{4d} point group symmetry as obtained from DFT using the LDA and GGA functionals together with the details of the optimized bond distances Tb-N(1) and Tb – N(2) and angles N(1) – Tb – (N1), N(2) – Tb – (N2) and N(1) – Tb – (N2).

Table S1. List of the experimental and calculated bond distances and angles of TbPc$_2$. The employed DFT functionals are indicated in the Table.

Bond distance Tb – N(1) EXP. 2.401 Å, 2.407 Å, 2.408 Å and 2.421 Å LDA. 2.392 Å GGA. 2.449 Å	Bond distance Tb – N(2) EXP. 2.397 Å, 2.405 Å, 2.408 Å and 2. 426 Å LDA. 2.392 Å GGA. 2.449 Å
Angle N(1) – Tb – N(1) EXP. 69.94°, 70.44°, 70.50° and 70.83° LDA. 71.18° GGA. 70.46°	Angle N(2) – Tb – N(2) EXP. 69.92°, 70.08°, 70.17° and 71.04° LDA. 71.18° GGA. 70.46°
Angle N(1) – Tb – N(2) EXP. 81.05°, 84.99°, 80.92°, 83.66°, 80.24°, 83.49°, 80.10° and 84.62 ° LDA. 81.00° GGA. 82.18°	

Table S2. Optimized atomic Cartesian coordinates (in Å) of TbPc$_2$ belonging to the D_{4d} point group calculated from DFT employing the LDA and GGA functionals.

	GGA				LDA		
Tb	0	0	0	Tb	0	0	0
N	1.412583	1.412582	-1.416323	N	1.819074	0.753485	-1.358829
N	1.412582	-1.412583	-1.416323	N	0.753485	-1.819074	-1.358829
N	-1.412582	1.412583	-1.416323	N	-0.753485	1.819074	-1.358829
N	-1.412583	-1.412582	-1.416323	N	-1.819074	-0.753485	-1.358829
N	1.997693	0	1.416323	N	1.819074	-0.753485	1.358829
N	0	-1.997693	1.416323	N	-0.753485	-1.819074	1.358829
N	0	1.997693	1.416323	N	0.753485	1.819074	1.358829
N	-1.997693	0	1.416323	N	-1.819074	0.753485	1.358829
C	2.746144	1.174361	-1.649676	C	2.958336	0.03213	-1.541438
C	-2.746144	-1.174361	-1.649676	C	-2.958336	-0.03213	-1.541438
C	-1.174361	2.746144	-1.649676	C	-0.03213	2.958336	-1.541438
C	1.174361	-2.746144	-1.649676	C	0.03213	-2.958336	-1.541438
C	2.772216	-1.11142	1.649676	C	2.114579	-2.069141	1.541438
C	1.111419	-2.772216	1.649676	C	-0.03213	-2.958336	1.541438
C	2.772216	1.111419	1.649676	C	2.958336	-0.03213	1.541438
C	-1.111419	2.772216	1.649676	C	0.03213	2.958336	1.541438
C	-2.772216	1.11142	1.649676	C	-2.114579	2.069141	1.541438
C	-2.772216	-1.111419	1.649676	C	-2.958336	0.03213	1.541438
C	1.11142	2.772216	1.649676	C	2.069141	2.114579	1.541438
C	-1.11142	-2.772216	1.649676	C	-2.069141	-2.114579	1.541438
C	2.746145	-1.174361	-1.649676	C	2.069141	-2.114579	-1.541438
C	1.174361	2.746145	-1.649676	C	2.114579	2.069141	-1.541438
C	-2.746145	1.174361	-1.649676	C	-2.069141	2.114579	-1.541438
C	-1.174361	-2.746145	-1.649676	C	-2.114579	-2.069141	-1.541438
N	2.385911	-2.385911	1.709644	N	1.279774	-3.089649	1.587428
N	-2.385911	2.385911	1.709644	N	-1.279774	3.089649	1.587428
N	2.385911	2.385911	1.709644	N	3.089649	1.279774	1.587428
N	-2.385911	-2.385911	1.709644	N	-3.089649	-1.279774	1.587428
N	3.374188	0	-1.709644	N	3.089649	-1.279774	-1.587428
N	-3.374188	0	-1.709644	N	-3.089649	1.279774	-1.587428
N	0	3.374188	-1.709644	N	1.279774	3.089649	-1.587428
N	0	-3.374188	-1.709644	N	-1.279774	-3.089649	-1.587428
C	3.431368	2.436676	-1.948933	C	4.072286	0.930886	-1.759023
C	2.436676	3.431368	-1.948933	C	3.537776	2.221305	-1.759023
C	-3.431368	2.436676	-1.948933	C	-2.221305	3.537776	-1.759023
C	3.431368	-2.436676	-1.948933	C	2.221305	-3.537776	-1.759023
C	2.436676	-3.431368	-1.948933	C	0.930886	-4.072286	-1.759023
C	-2.436676	-3.431368	-1.948933	C	-3.537776	-2.221305	-1.759023
C	-3.431368	-2.436676	-1.948933	C	-4.072286	-0.930886	-1.759023
C	-2.436676	3.431368	-1.948933	C	-0.930886	4.072286	-1.759023
C	4.149334	-0.703353	1.948933	C	3.537776	-2.221305	1.759023
C	4.149333	0.703354	1.948933	C	4.072286	-0.930886	1.759023
C	-0.703354	4.149333	1.948933	C	0.930886	4.072286	1.759023
C	0.703354	-4.149333	1.948933	C	-0.930886	-4.072286	1.759023
C	-0.703353	-4.149334	1.948933	C	-2.221305	-3.537776	1.759023
C	-4.149333	-0.703354	1.948933	C	-4.072286	0.930886	1.759023
C	-4.149334	0.703353	1.948933	C	-3.537776	2.221305	1.759023
C	0.703353	4.149334	1.948933	C	2.221305	3.537776	1.759023
C	5.307317	-1.425906	2.232323	C	4.341574	-3.330117	1.948951
C	5.307318	1.425906	2.232323	C	5.424705	-0.715208	1.948951
C	1.425906	-5.307318	2.232323	C	-0.715208	-5.424705	1.948951
C	-1.425906	5.307318	2.232323	C	0.715208	5.424705	1.948951
C	-1.425906	-5.307317	2.232323	C	-3.330117	-4.341574	1.948951
C	1.425906	5.307317	2.232323	C	3.330117	4.341574	1.948951
C	-5.307318	-1.425906	2.232323	C	-5.424705	0.715208	1.948951
C	-5.307317	1.425906	2.232323	C	-4.341574	3.330117	1.948951

C	4.761108	2.744572	-2.232323	C	5.424705	0.715208	-1.948951
C	2.744572	4.761108	-2.232323	C	4.341574	3.330117	-1.948951
C	4.761108	-2.744572	-2.232323	C	3.330117	-4.341574	-1.948951
C	-4.761108	2.744572	-2.232323	C	-3.330117	4.341574	-1.948951
C	2.744572	-4.761108	-2.232323	C	0.715208	-5.424705	-1.948951
C	-2.744572	4.761108	-2.232323	C	-0.715208	5.424705	-1.948951
C	-2.744572	-4.761108	-2.232323	C	-4.341574	-3.330117	-1.948951
C	-4.761108	-2.744572	-2.232323	C	-5.424705	-0.715208	-1.948951
H	-5.524129	1.966088	-2.241781	H	-4.332265	3.903411	-1.945822
H	1.966088	5.524129	-2.241781	H	3.903411	4.332265	-1.945822
H	5.524129	-1.966088	-2.241781	H	4.332265	-3.903411	-1.945822
H	-1.966088	-5.524129	-2.241781	H	-3.903411	-4.332265	-1.945822
H	5.296383	-2.515916	2.241781	H	3.903411	-4.332265	1.945822
H	-2.515915	5.296383	2.241781	H	-0.303246	5.823502	1.945822
H	5.296383	2.515915	2.241781	H	5.823502	0.303246	1.945822
H	2.515915	-5.296383	2.241781	H	0.303246	-5.823502	1.945822
H	-2.515916	-5.296383	2.241781	H	-4.332265	-3.903411	1.945822
H	2.515916	5.296383	2.241781	H	4.332265	3.903411	1.945822
H	-5.296383	2.515916	2.241781	H	-3.903411	4.332265	1.945822
H	-5.296383	-2.515915	2.241781	H	-5.823502	-0.303246	1.945822
H	5.524129	1.966088	-2.241781	H	5.823502	-0.303246	-1.945822
H	1.966088	-5.524129	-2.241781	H	-0.303246	-5.823502	-1.945822
H	-1.966088	5.524129	-2.241781	H	0.303246	5.823502	-1.945822
H	-5.524129	-1.966088	-2.241781	H	-5.823502	0.303246	-1.945822
C	6.47611	-0.702956	2.494803	C	5.698597	-3.116422	2.127887
C	6.47611	0.702956	2.494803	C	6.233159	-1.825873	2.127887
C	0.702956	-6.47611	2.494803	C	-1.825873	-6.233159	2.127887
C	-0.702956	-6.47611	2.494803	C	-3.116422	-5.698597	2.127887
C	-0.702956	6.47611	2.494803	C	1.825873	6.233159	2.127887
C	0.702956	6.47611	2.494803	C	3.116422	5.698597	2.127887
C	-6.47611	0.702956	2.494803	C	-5.698597	3.116422	2.127887
C	-6.47611	-0.702956	2.494803	C	-6.233159	1.825873	2.127887
C	5.076366	4.082236	-2.494803	C	6.233159	1.825873	-2.127887
C	4.082236	5.076367	-2.494803	C	5.698597	3.116422	-2.127887
C	5.076367	-4.082236	-2.494803	C	3.116422	-5.698597	-2.127887
C	4.082236	-5.076366	-2.494803	C	1.825873	-6.233159	-2.127887
C	-5.076367	4.082236	-2.494803	C	-3.116422	5.698597	-2.127887
C	-4.082236	5.076366	-2.494803	C	-1.825873	6.233159	-2.127887
C	-5.076366	-4.082236	-2.494803	C	-6.233159	-1.825873	-2.127887
C	-4.082236	-5.076367	-2.494803	C	-5.698597	-3.116422	-2.127887
H	6.109416	4.360985	-2.708653	H	7.309682	1.694851	-2.271095
H	4.360986	6.109417	-2.708653	H	6.367166	3.970285	-2.271095
H	6.109417	-4.360986	-2.708653	H	3.970285	-6.367166	-2.271095
H	-6.109417	4.360986	-2.708653	H	-3.970285	6.367166	-2.271095
H	4.360985	-6.109416	-2.708653	H	1.694851	-7.309682	-2.271095
H	-4.360985	6.109416	-2.708653	H	-1.694851	7.309682	-2.271095
H	-4.360986	-6.109417	-2.708653	H	-6.367166	-3.970285	-2.271095
H	-6.109416	-4.360985	-2.708653	H	-7.309682	-1.694851	-2.271095
H	7.403693	-1.236327	2.708653	H	6.367166	-3.970285	2.271095
H	7.403692	1.236327	2.708653	H	7.309682	-1.694851	2.271095
H	1.236327	-7.403692	2.708653	H	-1.694851	-7.309682	2.271095
H	-1.236327	7.403692	2.708653	H	1.694851	7.309682	2.271095
H	-1.236327	-7.403693	2.708653	H	-3.970285	-6.367166	2.271095
H	1.236327	7.403693	2.708653	H	3.970285	6.367166	2.271095
H	-7.403692	-1.236327	2.708653	H	-7.309682	1.694851	2.271095
H	-7.403693	1.236327	2.708653	H	-6.367166	3.970285	2.271095

Table S3. Kohn-Sham orbital energy levels (irrep) of TbPc$_2$ with Tb $4f^8$ and $3d^94f^9$ electron configurations, showing the calculated energy values (Eng in eV), the occupation scheme that are imposed in the DFT calculation (Occ.) and the percentage character of the Tb atomic orbitals (Tb Char.)

#	irrep	Tb $4f^8$			Tb $3d^94f^9$		
		Eng.	Occ.	Tb Char.	Eng.	Occ.	Tb Char.
13	a$_2$	-4.442	1		-4.436	1	
36	e$_2$	-4.655	2.28	91.83 % $4f_{xyz}$ & 91.83 % $4f_{z(x^2-y^2)}$	-5.125	2.58	87.03 % $4f_{xyz}$ & 87.03 % $4f_{z(x^2-y^2)}$
26	b$_2$	-4.684	1.14	92.93 % $4f_{z^3}$	-5.137	1.29	87.55 % $4f_{z^3}$
38	e$_1$	-4.719	2.28	94.86 % $4f_{z^2x}$ & 94.86 % $4f_{z^2y}$	-5.187	2.58	92.10 % $4f_{z^2x}$ & 92.10 % $4f_{z^2y}$
36	e$_3$	-4.858	2.28	96.83 % $4f_{x(x^2-3y^2)}$ & 96.83 % $4f_{y(3x^2-y^2)}$	-5.362	2.58	94.33 % $4f_{x(x^2-3y^2)}$ & 94.33 % $4f_{y(3x^2-y^2)}$
13	b$_1$	-4.942	2		-4.936	2	
35	e$_2$	-5.925	4		-5.924	4	
25	b$_2$	-5.933	2		-5.939	2	
34	e$_2$	-5.982	4		-5.974	4	
35	e$_3$	-6.005	4		-6.003	4	
28	a1	-6.024	2		-6.010	2	
37	e$_1$	-6.121	4		-6.119	4	
…							
4	a$_1$	-1233.904	2	100 % $3d_{z^2}$	-1270.086	1.80	99.99 % $3d_{z^2}$
1	e$_3$	-1233.905	4	100 % $3d_{xz}$ & 100 % $3d_{yz}$	-1270.094	3.60	100 % $3d_{xz}$ & 100 % $3d_{yz}$
1	e$_2$	-1233.956	4	100 % $3d_{x^2-y^2}$ & 100 % $3d_{xy}$	-1270.165	3.60	100 % $3d_{x^2-y^2}$ & 100 % $3d_{xy}$

Table S4. Calculated energy gap parameter (ΔE_{av}), Slater-Condon integrals (F^k) and spin-orbit coupling constants (ζ) (in eV) for configuration $3d^{10}4f^8$ of Tb^{3+} ion in the complex TbPc$_2$ obtained from DFT using the GGA functional.

	Tb^{3+}
	$3d^{10}4f^8$
$F^2(4f,4f)$	11.5534
$F^4(4f,4f)$	7.2062
$F^6(4f,4f)$	5.1718
ζ_{4f}	0.2022

Table S5. Calculated ligand-field (H_{LF}) matrix elements for $4f$ orbitals of Tb^{3+} ion (in eV) within configuration $3d^{10}4f^8$ in the complex TbPc$_2$ with D_{4d} symmetry obtained from DFT using the GGA functional.

	$4f_{y(3x^2-y^2)}$	$4f_{xyz}$	$4f_{z^2y}$	$4f_{z^3}$	$4f_{z^2x}$	$4f_{z(x^2-y^2)}$	$4f_{x(x^2-3y^2)}$
$|4f,e_3\rangle$	-0.1221	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$|4f,e_2\rangle$	0.0000	0.0801	0.0000	0.0000	0.0000	0.0000	0.0000
$|4f,e_1\rangle$	0.0000	0.0000	0.0164	0.0000	0.0000	0.0000	0.0000
$|4f,b_2\rangle$	0.0000	0.0000	0.0000	0.0512	0.0000	0.0000	0.0000
$|4f,e_1\rangle$	0.0000	0.0000	0.0000	0.0000	0.0164	0.0000	0.0000
$|4f,e_2\rangle$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0801	0.0000
$|4f,e_3\rangle$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1221

Table S6. Calculated energy gap parameter (ΔE_{av}), Slater-Condon integrals (F^k and G^k) and spin-orbit coupling constants (ζ) (in eV) for configuration $3d^94f^9$ of Tb^{3+} ion in the complex TbPc$_2$ obtained from DFT using the GGA functional.

	Tb^{3+}
	$3d^94f^9$
$F^2(4f,4f)$	10.4626
$F^4(4f,4f)$	6.5360
$F^6(4f,4f)$	4.6937
ΔE_{av}	1247.1
$G^1(3d,4f)$	5.5597
$G^3(3d,4f)$	3.2941
$G^5(3d,4f)$	2.2857
$F^2(3d,4f)$	8.0298
$F^4(3d,4f)$	3.7302
ζ_{3d}	13.4275
ζ_{4f}	0.2055

Table S7. Calculated ligand-field (H_{LF}) matrix elements for the merged $3d$ and $4f$ orbitals of Tb^{3+} ion (in eV) within configuration $3d^9 4f^9$ in the complex TbPc$_2$ with D_{4d} symmetry obtained from DFT using the GGA functional.

	$3d_{xy}$	$3d_{yz}$	$3d_{z^2}$	$3d_{xz}$	$3d_{x^2-y^2}$	$4f_{y(3x^2-y^2)}$	$4f_{xyz}$	$4f_{z^2y}$	$4f_{z^3}$	$4f_{z^2x}$	$4f_{z(x^2-y^2)}$	$4f_{x(x^2-3y^2)}$
$\lvert 3d, e_2 \rangle$	-0.0443	0.0000	0.0000	0.0000	0.0000	0.0000	0.27E-6	0.0000	0.0000	0.0000	0.0000	0.0000
$\lvert 3d, e_3 \rangle$	0.0000	0.0269	0.0000	0.0000	0.0000	0.10E-4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$\lvert 3d, a_1 \rangle$	0.0000	0.0000	0.0349	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$\lvert 3d, e_3 \rangle$	0.0000	0.0000	0.0000	0.0269	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.10E-4
$\lvert 3d, e_2 \rangle$	0.0000	0.0000	0.0000	0.0000	-0.0443	0.0000	0.0000	0.0000	0.0000	0.0000	-0.27E-6	0.0000
$\lvert 4f, e_3 \rangle$	0.0000	0.10E-4	0.0000	0.0000	0.0000	-0.1498	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$\lvert 4f, e_2 \rangle$	0.27E-6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0873	0.0000	0.0000	0.0000	0.0000	0.0000
$\lvert 4f, e_1 \rangle$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0249	0.0000	0.0000	0.0000	0.0000
$\lvert 4f, b_2 \rangle$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0752	0.0000	0.0000	0.0000
$\lvert 4f, e_1 \rangle$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0249	0.0000	0.0000
$\lvert 4f, e_2 \rangle$	0.0000	0.0000	0.0000	0.0000	-0.27E-6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0873	0.0000
$\lvert 4f, e_3 \rangle$	0.0000	0.0000	0.0000	-0.10E-4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1498

Table S8. Calculated energy levels (in cm^{-1}) of the ligand-field manifold of the ground state atomic multiplet of Tb^{3+} ion (i.e. $^7F_6$) within configuration $3d^{10}4f^8$ in the complex TbPc$_2$, obtained from DFT calculation using the GGA functional, together with their degeneracy (multiplicity) and their characterization with respect to the $\langle S^2 \rangle$, $\langle L^2 \rangle$ and $\langle J^2 \rangle$ expectation values, as output of the LFDFT calculation.

Multiplicity	Energy [cm^{-1}]	S(S+1)	L(L+1)	J(J+1)
2	0.000	8.701	9.304	36.000
2	510.516	4.601	8.150	25.000
2	911.431	2.414	5.985	16.000
2	1146.945	1.510	3.137	9.000
2	1232.283	0.831	1.184	4.000
2	1251.565	0.231	0.270	1.000
1	1254.029	0.000	0.000	0.000

Table S9. Selected energy levels (in eV) of the ligand-field manifold of the excited state multiplets of Tb^{3+} ion within configuration $3d^94f^9$ in the complex TbPc$_2$, obtained from DFT calculation using the GGA functional, together with their degeneracy (multiplicity), their characterization with respect to the $\langle S^2 \rangle$, $\langle L^2 \rangle$ and $\langle J^2 \rangle$ expectation values and the calculated transition probabilities vis-à-vis the initial state listed in Table S1, as output of the LFDFT calculation. The energy shift of -3.1 eV was not applied here.

Multiplicity	Energy [eV]	S(S+1)	L(L+1)	J(J+1)	$\langle i\|x\|f\rangle^2$	$\langle i\|y\|f\rangle^2$	$\langle i\|z\|f\rangle^2$
2	1233.606423	4.285	8.584	25.000	0.000123	0.000123	0.000000
2	1233.701650	4.025	24.937	49.000	0.000118	0.000118	0.000000
2	1233.708734	2.445	29.556	49.000	0.000099	0.000099	0.000000
2	1233.742123	5.363	21.941	49.000	0.008697	0.008697	0.000000
2	1233.811495	4.003	15.994	36.000	0.000000	0.000000	0.002281
2	1233.825473	3.087	10.517	25.000	0.000175	0.000175	0.000000
2	1234.025905	4.392	15.244	36.000	0.000000	0.000000	0.002150
2	1234.080992	2.441	11.817	25.000	0.000284	0.000284	0.000000
2	1234.347646	2.461	19.637	36.000	0.000000	0.000000	0.001524
2	1234.352160	1.726	13.587	25.000	0.000073	0.000073	0.000000
2	1234.356981	2.879	28.125	49.000	0.005018	0.005018	0.000000
2	1234.497543	1.432	14.467	25.000	0.000478	0.000478	0.000000
2	1234.523648	1.286	14.947	25.000	0.000086	0.000086	0.000000
2	1234.545251	1.486	22.858	36.000	0.000000	0.000000	0.000734
2	1234.557286	2.475	29.449	49.000	0.003500	0.003500	0.000000
2	1234.681664	3.677	25.830	49.000	0.000685	0.000685	0.000000
2	1234.689256	2.892	18.485	36.000	0.000000	0.000000	0.000221
2	1235.134731	1.938	13.017	25.000	0.000138	0.000138	0.000000
2	1235.161761	2.805	18.706	36.000	0.000000	0.000000	0.001227
2	1235.189594	1.645	22.255	36.000	0.000000	0.000000	0.000215
2	1235.287300	0.976	16.097	25.000	0.000157	0.000157	0.000000
2	1235.295644	0.980	25.100	36.000	0.000000	0.000000	0.004194
2	1235.346359	3.806	25.494	49.000	0.010417	0.010417	0.000000
2	1235.346901	2.140	20.586	36.000	0.000000	0.000000	0.000900
2	1235.458590	0.543	18.172	25.000	0.000452	0.000452	0.000000
2	1235.707457	1.993	12.876	25.000	0.000133	0.000133	0.000000
2	1235.742049	3.169	17.807	36.000	0.000000	0.000000	0.001606
2	1235.762597	2.089	30.853	49.000	0.006544	0.006544	0.000000
2	1235.796214	1.977	21.104	36.000	0.000000	0.000000	0.002865
2	1235.811101	1.576	14.022	25.000	0.000239	0.000239	0.000000
2	1235.912745	2.188	12.397	25.000	0.000684	0.000684	0.000000
2	1235.959759	0.766	34.517	25.000	0.000213	0.000213	0.000000
2	1236.117267	1.527	14.170	25.000	0.000067	0.000067	0.000000
2	1236.123347	2.370	19.896	36.000	0.000000	0.000000	0.001207
2	1236.151000	3.263	26.975	49.000	0.001820	0.001820	0.000000
2	1236.186965	1.419	14.505	25.000	0.001376	0.001376	0.000000
2	1236.339315	0.207	20.657	25.000	0.000054	0.000054	0.000000
2	1236.344877	0.369	29.082	36.000	0.000000	0.000000	0.006536
2	1236.350422	0.314	19.707	25.000	0.000443	0.000443	0.000000
2	1236.353257	0.317	29.565	36.000	0.000000	0.000000	0.001169
2	1236.499538	1.718	13.612	25.000	0.000230	0.000230	0.000000
2	1236.530973	1.932	21.254	36.000	0.000000	0.000000	0.010581
2	1236.566038	0.695	26.690	36.000	0.000000	0.000000	0.005980
2	1236.611770	0.676	26.809	36.000	0.000000	0.000000	0.000181
2	1236.647517	3.842	9.242	25.000	0.002931	0.002931	0.000000
2	1236.661969	4.164	15.677	36.000	0.000000	0.000000	0.119508
2	1236.726055	1.569	33.031	49.000	0.002868	0.002868	0.000000
2	1236.735088	2.894	10.881	25.000	0.009090	0.009090	0.000000
2	1236.750298	1.369	23.327	36.000	0.000000	0.000000	0.002324
2	1236.785652	0.769	16.999	25.000	0.001013	0.001013	0.000000
2	1236.866124	0.864	36.852	49.000	0.000052	0.000052	0.000000
2	1236.867734	0.005	24.324	25.000	0.000060	0.000060	0.000000
2	1236.962400	0.549	27.656	36.000	0.000000	0.000000	0.000638
2	1237.010985	0.613	38.650	49.000	0.000071	0.000071	0.000000

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2	1237.059632	1.399	33.839	49.000	0.000215	0.000215	0.000000
2	1237.065367	1.215	23.986	36.000	0.000000	0.000000	0.000317
2	1237.114643	0.381	40.739	49.000	0.000083	0.000083	0.000000
2	1237.119245	0.307	29.662	36.000	0.000000	0.000000	0.000139
2	1237.127307	0.894	16.437	25.000	0.000115	0.000115	0.000000
2	1237.134748	1.269	23.749	36.000	0.000000	0.000000	0.004790
2	1237.222969	2.857	28.192	49.000	0.012635	0.012635	0.000000
2	1237.232144	1.958	21.168	36.000	0.000000	0.000000	0.002257
2	1237.238528	2.249	12.252	25.000	0.011519	0.011519	0.000000
2	1237.243515	1.209	15.214	25.000	0.001878	0.001878	0.000000
2	1237.288459	0.696	38.014	49.000	0.000123	0.000123	0.000000
2	1237.294035	0.486	18.518	25.000	0.000206	0.000206	0.000000
2	1237.346185	0.386	19.172	25.000	0.001383	0.001383	0.000000
2	1237.359692	0.079	32.715	36.000	0.000000	0.000000	0.000392
2	1237.361878	0.156	21.203	25.000	0.002122	0.002122	0.000000
2	1237.387342	0.500	18.426	25.000	0.000622	0.000622	0.000000
2	1237.395845	0.598	27.320	36.000	0.000000	0.000000	0.002827
2	1237.403949	0.344	29.305	36.000	0.000000	0.000000	0.000608
2	1237.404282	0.518	39.444	49.000	0.002927	0.002927	0.000000
2	1237.417057	0.232	20.419	25.000	0.000058	0.000058	0.000000
2	1237.460005	0.166	31.278	36.000	0.000000	0.000000	0.000499
2	1237.471503	0.061	22.594	25.000	0.000059	0.000059	0.000000
2	1237.586728	0.051	33.345	36.000	0.000000	0.000000	0.002724
2	1237.604561	1.087	35.493	49.000	0.000052	0.000052	0.000000
2	1237.605492	0.956	25.223	36.000	0.000000	0.000000	0.000258
2	1237.605894	0.076	22.326	25.000	0.000568	0.000568	0.000000
2	1237.613919	0.149	21.286	25.000	0.000382	0.000382	0.000000
2	1237.668135	0.621	27.161	36.000	0.000000	0.000000	0.000213
2	1237.684301	0.642	38.424	49.000	0.000764	0.000764	0.000000
2	1237.717212	0.730	17.187	25.000	0.001122	0.001122	0.000000
2	1237.725645	0.651	26.967	36.000	0.000000	0.000000	0.000146
2	1237.737962	1.202	15.240	25.000	0.005599	0.005599	0.000000
2	1237.744439	0.602	17.844	25.000	0.000226	0.000226	0.000000
2	1237.761199	0.818	25.967	36.000	0.000000	0.000000	0.004505
2	1237.789520	0.285	29.875	36.000	0.000000	0.000000	0.000176
2	1237.801234	0.163	31.325	36.000	0.000000	0.000000	0.000450
2	1237.804088	0.047	22.869	25.000	0.000229	0.000229	0.000000
2	1237.850428	0.013	34.635	36.000	0.000000	0.000000	0.000243
2	1237.901697	0.053	45.830	49.000	0.000451	0.000451	0.000000
2	1237.922859	0.327	19.609	25.000	0.000171	0.000171	0.000000
2	1237.932618	0.035	46.427	49.000	0.000138	0.000138	0.000000
2	1238.077087	0.556	27.608	36.000	0.000000	0.000000	0.001661
2	1238.085762	0.263	20.135	25.000	0.000142	0.000142	0.000000
2	1238.091960	0.803	37.255	49.000	0.001089	0.001089	0.000000
2	1238.134320	0.373	19.268	25.000	0.003110	0.003110	0.000000
2	1238.188104	0.416	40.386	49.000	0.000123	0.000123	0.000000
2	1238.242625	0.141	21.381	25.000	0.000078	0.000078	0.000000
2	1238.314626	1.398	23.210	36.000	0.000000	0.000000	0.001848
2	1238.317676	1.327	14.807	25.000	0.001027	0.001027	0.000000
2	1238.325076	0.185	43.158	49.000	0.000132	0.000132	0.000000
2	1238.331938	0.533	27.774	36.000	0.000000	0.000000	0.000295
2	1238.343183	0.247	20.277	25.000	0.000186	0.000186	0.000000
2	1238.410295	0.328	19.603	25.000	0.000404	0.000404	0.000000
2	1238.410463	0.318	29.547	36.000	0.000000	0.000000	0.000195
2	1238.415566	0.357	40.988	49.000	0.000063	0.000063	0.000000
2	1238.448357	2.210	12.343	25.000	0.003589	0.003589	0.000000
2	1238.464140	0.547	18.151	25.000	0.003063	0.003063	0.000000
2	1238.478170	2.751	18.849	36.000	0.000000	0.000000	0.006737
2	1238.488630	0.380	19.218	25.000	0.002699	0.002699	0.000000
2	1238.556386	0.110	21.800	25.000	0.000076	0.000076	0.000000
2	1238.558700	0.086	22.159	25.000	0.000114	0.000114	0.000000
2	1238.590033	0.196	30.878	36.000	0.000000	0.000000	0.000590
2	1238.611861	0.037	23.104	25.000	0.000220	0.000220	0.000000
2	1238.655578	0.468	18.629	25.000	0.000455	0.000455	0.000000
2	1238.689707	1.697	13.669	25.000	0.008200	0.008200	0.000000
2	1238.738115	0.042	22.998	25.000	0.000182	0.000182	0.000000
2	1238.757400	0.143	43.850	49.000	0.000147	0.000147	0.000000
2	1238.816010	0.136	21.451	25.000	0.000385	0.000385	0.000000
2	1238.883617	0.992	16.033	25.000	0.024912	0.024912	0.000000
2	1238.886777	1.881	13.166	25.000	0.039718	0.039718	0.000000
2	1238.899391	0.253	20.223	25.000	0.001179	0.001179	0.000000
2	1238.915172	0.045	33.494	36.000	0.000000	0.000000	0.000965
2	1238.941190	0.117	21.701	25.000	0.003077	0.003077	0.000000
2	1238.995640	0.585	17.938	25.000	0.000954	0.000954	0.000000
2	1239.003725	0.982	25.091	36.000	0.000000	0.000000	0.000404
2	1239.075880	0.110	21.797	25.000	0.000157	0.000157	0.000000
2	1239.079467	0.168	21.075	25.000	0.000373	0.000373	0.000000
2	1239.115962	0.127	21.558	25.000	0.000135	0.000135	0.000000
2	1239.118894	0.328	41.313	49.000	0.000067	0.000067	0.000000
2	1239.124521	0.000	49.217	49.000	0.000065	0.000065	0.000000
2	1239.189043	0.382	28.963	36.000	0.000000	0.000000	0.002526
2	1239.191242	0.071	22.409	25.000	0.000069	0.000069	0.000000
2	1239.229527	0.079	22.264	25.000	0.000109	0.000109	0.000000
2	1239.265009	0.036	33.759	36.000	0.000000	0.000000	0.001083
2	1239.283294	0.218	20.551	25.000	0.000153	0.000153	0.000000
2	1239.285130	0.171	31.208	36.000	0.000000	0.000000	0.000168
2	1239.302879	0.654	38.335	49.000	0.000127	0.000127	0.000000
2	1239.311747	0.668	26.863	36.000	0.000000	0.000000	0.002677

2	1239.311878	0.304	19.793	25.000	0.000135	0.000135	0.000000
2	1239.335662	0.040	33.647	36.000	0.000000	0.000000	0.000959
2	1239.349457	0.079	22.266	25.000	0.002839	0.002839	0.000000
2	1239.350010	0.326	29.471	36.000	0.000000	0.000000	0.001027
2	1239.362175	0.256	20.193	25.000	0.000834	0.000834	0.000000
2	1239.377151	0.332	29.414	36.000	0.000000	0.000000	0.006601
2	1239.379517	0.189	20.844	25.000	0.000119	0.000119	0.000000
2	1239.403414	0.210	20.628	25.000	0.000642	0.000642	0.000000
2	1239.529943	0.399	19.081	25.000	0.000622	0.000622	0.000000
2	1239.665124	0.133	31.756	36.000	0.000000	0.000000	0.000172
2	1239.676045	0.791	16.895	25.000	0.000072	0.000072	0.000000
2	1239.705939	0.506	18.390	25.000	0.000463	0.000463	0.000000
2	1239.761385	0.066	22.493	25.000	0.000127	0.000127	0.000000
2	1239.763424	0.524	27.840	36.000	0.000000	0.000000	0.004014
2	1239.766501	0.138	31.685	36.000	0.000000	0.000000	0.001319
2	1239.779873	0.308	19.762	25.000	0.000365	0.000365	0.000000
2	1239.842664	0.096	21.994	25.000	0.000116	0.000116	0.000000
2	1239.853284	0.136	31.717	36.000	0.000000	0.000000	0.001098
2	1239.914054	0.376	19.244	25.000	0.000067	0.000067	0.000000
2	1240.019078	0.268	42.023	49.000	0.000422	0.000422	0.000000
2	1240.027194	0.002	24.613	25.000	0.000071	0.000071	0.000000
2	1240.042035	0.007	37.008	36.000	0.000000	0.000000	0.001066
2	1240.112035	0.265	42.056	49.000	0.000060	0.000060	0.000000
2	1240.145704	0.005	35.139	36.000	0.000000	0.000000	0.000242
2	1240.161325	0.124	44.200	49.000	0.000342	0.000342	0.000000
2	1240.322560	0.165	21.108	25.000	0.000387	0.000387	0.000000
2	1240.330004	0.237	42.424	49.000	0.000292	0.000292	0.000000
2	1240.333065	0.371	19.278	25.000	0.000364	0.000364	0.000000
2	1240.369073	0.531	39.332	49.000	0.001633	0.001633	0.000000
2	1240.372119	0.091	22.070	25.000	0.000115	0.000115	0.000000
2	1240.389732	0.266	30.082	36.000	0.000000	0.000000	0.000752
2	1240.418311	0.115	21.722	25.000	0.000062	0.000062	0.000000
2	1240.442076	0.274	20.040	25.000	0.000452	0.000452	0.000000
2	1240.452150	0.242	30.335	36.000	0.000000	0.000000	0.000556
2	1240.458257	0.105	21.864	25.000	0.000200	0.000200	0.000000
2	1240.472189	0.003	25.580	25.000	0.000281	0.000281	0.000000
2	1240.473192	0.265	42.058	49.000	0.000338	0.000338	0.000000
2	1240.477267	0.357	29.187	36.000	0.000000	0.000000	0.002466
2	1240.581412	0.283	41.837	49.000	0.000523	0.000523	0.000000
2	1240.583362	0.137	31.696	36.000	0.000000	0.000000	0.000229
2	1240.586779	0.206	20.671	25.000	0.000158	0.000158	0.000000
2	1240.591128	0.175	20.996	25.000	0.000261	0.000261	0.000000
2	1240.593348	0.239	20.346	25.000	0.000237	0.000237	0.000000
2	1240.593853	0.191	30.947	36.000	0.000000	0.000000	0.000361
2	1240.602629	0.713	17.270	25.000	0.000869	0.000869	0.000000
2	1240.639800	0.070	22.417	25.000	0.000069	0.000069	0.000000
2	1240.645834	0.110	32.127	36.000	0.000000	0.000000	0.002052
2	1240.712268	0.075	45.240	49.000	0.000192	0.000192	0.000000
2	1240.720667	0.416	28.675	36.000	0.000000	0.000000	0.000120
2	1240.721439	0.255	42.182	49.000	0.000326	0.000326	0.000000
2	1240.734071	0.040	33.646	36.000	0.000000	0.000000	0.000216
2	1240.736800	0.043	33.546	36.000	0.000000	0.000000	0.000215
2	1240.757929	0.064	45.533	49.000	0.000101	0.000101	0.000000
2	1240.765167	0.238	42.405	49.000	0.001093	0.001093	0.000000
2	1240.772177	0.563	39.057	49.000	0.000680	0.000680	0.000000
2	1240.818779	0.167	31.267	36.000	0.000000	0.000000	0.000283
2	1240.833612	0.161	43.547	49.000	0.000501	0.000501	0.000000
2	1240.907488	0.259	42.137	49.000	0.000177	0.000177	0.000000
2	1240.915054	0.746	37.657	49.000	0.000404	0.000404	0.000000
2	1240.928398	0.089	32.501	36.000	0.000000	0.000000	0.000141
2	1240.930627	0.001	36.344	36.000	0.000000	0.000000	0.000376
2	1241.011266	0.283	29.895	36.000	0.000000	0.000000	0.000433
2	1241.017329	0.412	28.710	36.000	0.000000	0.000000	0.000272
2	1241.057405	0.133	21.487	25.000	0.000051	0.000051	0.000000
2	1241.073112	0.064	22.529	25.000	0.000145	0.000145	0.000000
2	1241.164298	0.044	22.957	25.000	0.000070	0.000070	0.000000
2	1241.289695	0.478	18.563	25.000	0.002736	0.002736	0.000000
2	1241.300563	0.393	19.126	25.000	0.000560	0.000560	0.000000
2	1241.302709	0.143	21.368	25.000	0.000071	0.000071	0.000000
2	1241.314309	0.163	21.127	25.000	0.000289	0.000289	0.000000
2	1241.321880	0.159	21.168	25.000	0.000086	0.000086	0.000000
2	1241.324048	0.201	30.820	36.000	0.000000	0.000000	0.000126
2	1241.355913	0.100	21.933	25.000	0.000258	0.000258	0.000000
2	1241.382417	0.055	33.248	36.000	0.000000	0.000000	0.000620
2	1241.384714	0.180	31.085	36.000	0.000000	0.000000	0.000885
2	1241.438059	0.029	23.318	25.000	0.000431	0.000431	0.000000
2	1241.521286	0.147	21.318	25.000	0.000093	0.000093	0.000000
2	1241.535305	0.183	31.051	36.000	0.000000	0.000000	0.001154
2	1241.550477	0.194	20.785	25.000	0.000915	0.000915	0.000000
2	1241.559653	0.233	30.439	36.000	0.000000	0.000000	0.000967
2	1241.577022	0.060	22.618	25.000	0.000915	0.000915	0.000000
2	1241.614193	0.690	26.721	36.000	0.000000	0.000000	0.000185
2	1241.642477	0.071	22.403	25.000	0.000245	0.000245	0.000000
2	1241.645518	0.272	30.016	36.000	0.000000	0.000000	0.000787
2	1241.657196	0.385	28.941	36.000	0.000000	0.000000	0.000535
2	1241.676998	0.398	19.091	25.000	0.000322	0.000322	0.000000
2	1241.712850	0.090	22.088	25.000	0.000149	0.000149	0.000000
2	1241.725005	0.158	21.188	25.000	0.000683	0.000683	0.000000

2	1241.736824	0.017	23.712	25.000	0.000355	0.000355	0.000000
2	1241.775712	0.094	22.021	25.000	0.000083	0.000083	0.000000
2	1241.790871	0.155	21.213	25.000	0.000532	0.000532	0.000000
2	1241.794567	0.348	19.448	25.000	0.000392	0.000392	0.000000
2	1241.921451	0.051	22.793	25.000	0.000098	0.000098	0.000000
2	1241.945225	0.290	19.907	25.000	0.000106	0.000106	0.000000
2	1241.967193	0.263	20.133	25.000	0.000312	0.000312	0.000000
2	1241.974005	0.247	20.276	25.000	0.000531	0.000531	0.000000
2	1242.023319	0.243	20.311	25.000	0.000344	0.000344	0.000000
2	1242.152845	0.009	34.858	36.000	0.000000	0.000000	0.000394
2	1242.232105	0.646	27.002	36.000	0.000000	0.000000	0.000633
2	1242.241749	0.078	22.289	25.000	0.000114	0.000114	0.000000
2	1242.287165	0.369	19.298	25.000	0.000130	0.000130	0.000000
2	1242.419465	0.120	31.964	36.000	0.000000	0.000000	0.000117
2	1242.444317	0.025	23.457	25.000	0.000151	0.000151	0.000000
2	1242.444731	0.090	32.490	36.000	0.000000	0.000000	0.001370
2	1242.467047	0.115	32.046	36.000	0.000000	0.000000	0.000362
2	1242.494324	0.090	32.484	36.000	0.000000	0.000000	0.000264
2	1242.519496	0.032	33.871	36.000	0.000000	0.000000	0.000231
2	1242.524311	0.318	19.680	25.000	0.000176	0.000176	0.000000
2	1242.533071	0.664	26.885	36.000	0.000000	0.000000	0.004016
2	1242.545196	0.365	29.120	36.000	0.000000	0.000000	0.000159
2	1242.554069	0.218	20.550	25.000	0.000396	0.000396	0.000000
2	1242.634456	0.298	41.661	49.000	0.000146	0.000146	0.000000
2	1242.644663	0.029	33.978	36.000	0.000000	0.000000	0.001012
2	1242.679828	0.748	37.641	49.000	0.000423	0.000423	0.000000
2	1242.721894	0.066	22.497	25.000	0.000155	0.000155	0.000000
2	1242.735723	0.172	31.192	36.000	0.000000	0.000000	0.000740
2	1242.738097	0.124	21.603	25.000	0.000111	0.000111	0.000000
2	1242.763819	0.376	29.019	36.000	0.000000	0.000000	0.000363
2	1242.781331	0.730	37.766	49.000	0.000089	0.000089	0.000000
2	1242.818502	0.089	22.112	25.000	0.000114	0.000114	0.000000
2	1242.856788	0.211	30.693	36.000	0.000000	0.000000	0.000727
2	1242.872332	0.415	40.397	49.000	0.000305	0.000305	0.000000
2	1242.902755	0.265	30.087	36.000	0.000000	0.000000	0.000337
2	1242.908068	0.094	22.034	25.000	0.000073	0.000073	0.000000
2	1242.922477	0.173	31.179	36.000	0.000000	0.000000	0.000679
2	1242.964182	0.152	31.476	36.000	0.000000	0.000000	0.000105
2	1242.968406	0.077	22.303	25.000	0.000074	0.000074	0.000000
2	1243.050660	0.613	38.651	49.000	0.000398	0.000398	0.000000
2	1243.155942	0.200	30.833	36.000	0.000000	0.000000	0.000122
2	1243.169490	0.148	21.302	25.000	0.000172	0.000172	0.000000
2	1243.173083	0.404	28.780	36.000	0.000000	0.000000	0.002177
2	1243.268979	0.087	22.139	25.000	0.000080	0.000080	0.000000
2	1243.303104	0.002	35.486	36.000	0.000000	0.000000	0.000148
2	1243.357729	0.010	24.010	25.000	0.000053	0.000053	0.000000
2	1243.380771	0.282	41.850	49.000	0.000058	0.000058	0.000000
2	1243.688240	0.149	31.521	36.000	0.000000	0.000000	0.000461
2	1243.760945	0.322	41.381	49.000	0.000075	0.000075	0.000000
2	1243.862798	0.064	22.536	25.000	0.000169	0.000169	0.000000
2	1243.870755	0.088	32.538	36.000	0.000000	0.000000	0.000397
2	1243.897640	1.175	24.168	36.000	0.000000	0.000000	0.000294
2	1243.927018	1.180	34.974	49.000	0.000721	0.000721	0.000000
2	1243.966585	0.529	39.342	49.000	0.000442	0.000442	0.000000
2	1243.994326	0.402	40.531	49.000	0.000065	0.000065	0.000000
2	1244.038409	0.200	30.827	36.000	0.000000	0.000000	0.000255
2	1244.040785	0.592	38.817	49.000	0.000108	0.000108	0.000000
2	1244.062445	0.397	28.834	36.000	0.000000	0.000000	0.000108
2	1244.185593	0.192	30.930	36.000	0.000000	0.000000	0.000297
2	1244.188746	0.135	21.460	25.000	0.000098	0.000098	0.000000
2	1244.286583	0.175	31.155	36.000	0.000000	0.000000	0.000264
2	1244.292013	0.129	44.100	49.000	0.000099	0.000099	0.000000
2	1244.364014	1.316	34.254	49.000	0.001032	0.001032	0.000000
2	1244.458926	0.137	31.701	36.000	0.000000	0.000000	0.000567
2	1244.593985	0.397	19.095	25.000	0.000090	0.000090	0.000000
2	1244.739402	0.214	20.588	25.000	0.000077	0.000077	0.000000
2	1244.746043	0.216	20.568	25.000	0.000076	0.000076	0.000000
2	1244.759828	0.237	30.395	36.000	0.000000	0.000000	0.000773
2	1245.083291	0.000	48.791	49.000	0.000089	0.000089	0.000000
2	1245.237720	0.172	21.025	25.000	0.000056	0.000056	0.000000
2	1245.254092	0.879	25.627	36.000	0.000000	0.000000	0.000488
2	1245.282167	0.446	18.769	25.000	0.000069	0.000069	0.000000
2	1245.478729	0.340	29.342	36.000	0.000000	0.000000	0.000100
2	1245.608645	0.374	40.817	49.000	0.000050	0.000050	0.000000
2	1245.977820	0.207	20.658	25.000	0.000079	0.000079	0.000000
2	1247.389390	0.334	41.248	49.000	0.000112	0.000112	0.000000
2	1247.421443	0.516	39.460	49.000	0.000195	0.000195	0.000000
2	1247.490108	0.152	43.686	49.000	0.000136	0.000136	0.000000
2	1247.820906	0.338	41.194	49.000	0.000067	0.000067	0.000000
2	1249.747369	0.482	39.765	49.000	0.000077	0.000077	0.000000
2	1267.816411	0.138	28.853	25.000	0.000066	0.000066	0.000000
1	1268.226275	0.569	27.520	36.000	0.000000	0.000000	0.000917
2	1268.239598	1.176	34.996	49.000	0.002053	0.002053	0.000000
2	1268.963892	3.134	10.431	25.000	0.010711	0.010711	0.000000
2	1269.296200	1.943	13.004	25.000	0.003417	0.003417	0.000000
2	1269.321897	3.542	16.957	36.000	0.000000	0.000000	0.028451
2	1269.400951	1.413	14.526	25.000	0.001454	0.001454	0.000000
2	1269.818281	1.108	15.581	25.000	0.000944	0.000944	0.000000

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2	1269.829463	3.214	17.702	36.000	0.000000	0.000000	0.050252
2	1269.855190	1.395	14.585	25.000	0.002775	0.002775	0.000000
2	1269.931693	3.293	26.889	49.000	0.019776	0.019776	0.000000
2	1269.946114	2.677	19.044	36.000	0.000000	0.000000	0.008124
2	1269.985050	2.943	10.787	25.000	0.001820	0.001820	0.000000
2	1270.350919	2.104	20.699	36.000	0.000000	0.000000	0.005951
2	1270.351345	1.423	14.493	25.000	0.000716	0.000716	0.000000
2	1270.634180	0.616	17.768	25.000	0.000275	0.000275	0.000000
2	1270.805865	1.258	50.715	36.000	0.000000	0.000000	0.000285
2	1270.969633	2.906	18.451	36.000	0.000000	0.000000	0.019773
2	1271.034027	1.484	14.302	25.000	0.001473	0.001473	0.000000
2	1271.078637	2.515	29.313	49.000	0.003749	0.003749	0.000000
2	1271.134023	0.967	16.134	25.000	0.000123	0.000123	0.000000
2	1271.180463	2.499	29.368	49.000	0.000101	0.000101	0.000000
2	1271.192247	1.472	22.915	36.000	0.000000	0.000000	0.000106
2	1271.206686	0.840	16.675	25.000	0.000092	0.000092	0.000000
2	1271.238608	0.104	21.878	25.000	0.000463	0.000463	0.000000
2	1271.258441	0.030	23.300	25.000	0.000142	0.000142	0.000000
2	1271.392671	0.870	62.930	49.000	0.000261	0.000261	0.000000
2	1271.551739	0.243	30.331	36.000	0.000000	0.000000	0.001688
2	1271.579291	0.163	21.125	25.000	0.000201	0.000201	0.000000
2	1271.822092	0.356	19.388	25.000	0.000162	0.000162	0.000000
2	1271.862888	0.102	32.267	36.000	0.000000	0.000000	0.000132
2	1271.872472	0.279	41.888	49.000	0.000410	0.000410	0.000000
2	1272.023287	2.841	10.985	25.000	0.000798	0.000798	0.000000
2	1272.228084	0.127	44.145	49.000	0.000082	0.000082	0.000000
2	1272.239898	0.257	56.354	49.000	0.000308	0.000308	0.000000
2	1272.258634	0.328	29.454	36.000	0.000000	0.000000	0.000330
2	1272.534236	0.473	28.217	36.000	0.000000	0.000000	0.000350
2	1272.563645	0.644	38.412	49.000	0.000170	0.000170	0.000000
2	1272.624873	0.003	25.579	25.000	0.000295	0.000295	0.000000
2	1272.658000	0.041	33.616	36.000	0.000000	0.000000	0.001125
2	1272.689275	1.099	35.422	49.000	0.004705	0.004705	0.000000
2	1272.692348	0.003	35.298	36.000	0.000000	0.000000	0.000421
2	1272.703368	0.470	28.247	36.000	0.000000	0.000000	0.000858
2	1272.708899	0.102	53.584	49.000	0.000384	0.000384	0.000000
2	1272.771326	0.035	51.646	49.000	0.000106	0.000106	0.000000
2	1272.775186	0.005	25.731	25.000	0.000080	0.000080	0.000000
2	1272.824054	0.005	25.684	25.000	0.000157	0.000157	0.000000
2	1273.015845	0.322	19.650	25.000	0.000070	0.000070	0.000000
2	1273.021625	0.245	20.300	25.000	0.000181	0.000181	0.000000
2	1273.027675	0.130	31.796	36.000	0.000000	0.000000	0.000635
2	1273.070757	0.183	43.190	49.000	0.001901	0.001901	0.000000
2	1273.098764	0.270	41.999	49.000	0.000755	0.000755	0.000000
2	1273.110650	0.507	27.966	36.000	0.000000	0.000000	0.000215
2	1273.110680	0.016	47.257	49.000	0.000317	0.000317	0.000000
2	1273.146639	0.078	22.287	25.000	0.000310	0.000310	0.000000
2	1273.163379	0.082	39.512	36.000	0.000000	0.000000	0.000316
2	1273.163991	0.118	44.313	49.000	0.000063	0.000063	0.000000
2	1273.185159	0.751	17.086	25.000	0.000696	0.000696	0.000000
2	1273.191467	0.391	19.140	25.000	0.000197	0.000197	0.000000
2	1273.290766	0.091	53.324	49.000	0.000239	0.000239	0.000000
2	1273.307768	0.059	45.668	49.000	0.000095	0.000095	0.000000
2	1273.330617	0.037	38.361	36.000	0.000000	0.000000	0.000150
2	1273.469063	0.036	33.757	36.000	0.000000	0.000000	0.000376
2	1273.490311	0.105	32.217	36.000	0.000000	0.000000	0.000421
2	1273.514585	0.044	46.119	49.000	0.000062	0.000062	0.000000
2	1273.616777	0.031	23.280	25.000	0.000050	0.000050	0.000000
2	1273.621574	0.039	33.681	36.000	0.000000	0.000000	0.000168
2	1273.624372	0.103	44.600	49.000	0.000253	0.000253	0.000000
2	1273.694496	0.120	31.956	36.000	0.000000	0.000000	0.000286
2	1273.710234	0.088	22.125	25.000	0.000300	0.000300	0.000000
2	1273.738692	0.078	32.729	36.000	0.000000	0.000000	0.000116
2	1273.836861	0.069	32.909	36.000	0.000000	0.000000	0.000149
2	1273.854008	0.081	32.665	36.000	0.000000	0.000000	0.000391
2	1273.867690	0.037	33.730	36.000	0.000000	0.000000	0.001558
2	1273.899264	0.038	33.702	36.000	0.000000	0.000000	0.000241
2	1274.127681	0.002	49.646	49.000	0.000054	0.000054	0.000000
2	1274.150743	0.081	22.241	25.000	0.000116	0.000116	0.000000
2	1274.377416	0.919	36.495	49.000	0.000659	0.000659	0.000000
2	1274.395413	0.542	27.704	36.000	0.000000	0.000000	0.000201
2	1274.585446	0.053	33.278	36.000	0.000000	0.000000	0.000701
2	1274.900229	0.435	28.521	36.000	0.000000	0.000000	0.000112
2	1274.952410	0.036	23.150	25.000	0.000084	0.000084	0.000000
2	1274.953613	0.014	37.432	36.000	0.000000	0.000000	0.000510
2	1275.046800	0.051	33.330	36.000	0.000000	0.000000	0.000342
2	1275.120956	0.000	36.020	36.000	0.000000	0.000000	0.000128
2	1275.257602	0.399	40.553	49.000	0.000156	0.000156	0.000000
2	1275.670139	0.023	37.863	36.000	0.000000	0.000000	0.000115
2	1275.676825	0.002	35.441	36.000	0.000000	0.000000	0.000475
2	1275.872244	0.263	20.135	25.000	0.000052	0.000052	0.000000
2	1276.987726	0.170	43.395	49.000	0.000056	0.000056	0.000000
2	1277.815976	0.355	41.009	49.000	0.000114	0.000114	0.000000
2	1278.063496	0.274	41.949	49.000	0.000105	0.000105	0.000000
2	1278.351788	0.207	42.834	49.000	0.000103	0.000103	0.000000

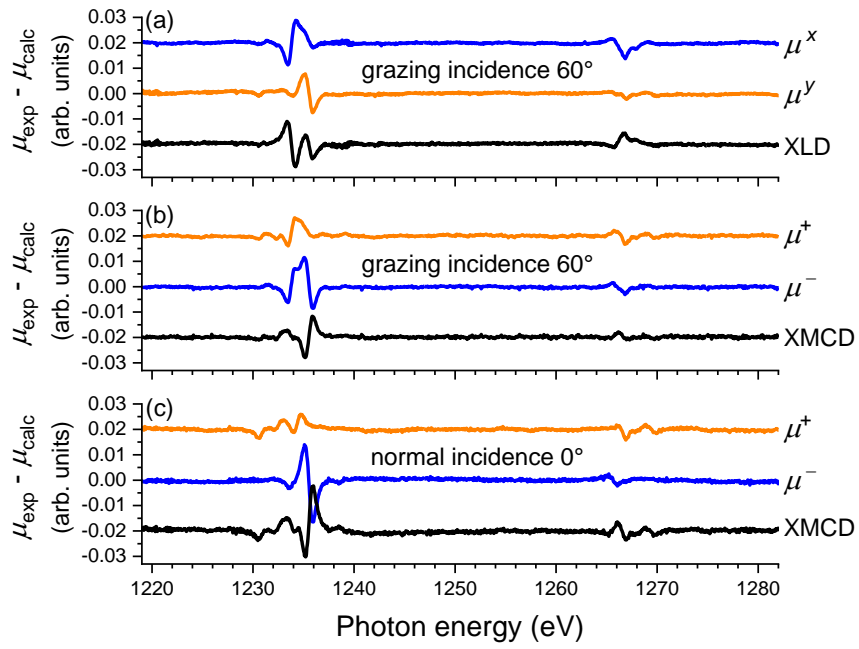**Figure S2.** Residuals of the polarized X-ray spectra calculated as μ_{exp} - μ_{calc}. (a) Linear polarization at grazing incidence as shown in Figure 3 of the main text. (b,c) Circular polarization at (b) grazing and (c) normal incidence as shown in Figure 2 of the main text.