ELECTRONIC SUPPLEMENTARY INFORMATION:

Ab initio quantum–chemical computations of the absorption cross sections in HgX_2 and HgXY (X, Y=Cl, Br, and I): Molecules of interest on the Earth's atmosphere

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CONTENTS

S.I. Basic information on the HgX_2 and HgXY equilibrium structures 3

S.II. Additional Tables 5

A. Allowed vertical electronic transitions of HgX_2 and HgXY 5

B. Multiconfigurational nature of the spin–free states of HgX_2 and HgXY 11

C. Extended data on the energetics of the excited states of HgX_2 and HgXY 17

S.III. Benchmark on the absorption cross section simulations 21

A. Equilibrium structures used in the generation of the Wigner distributions 21

B. Number of sampled geometries 23

S.IV. Simulated UV–Vis absorption cross sections of HgXY 25

References 29

S.I. BASIC INFORMATION ON THE HgX_2 AND HGXY EQUILIBRIUM STRUCTURES

TABLE S.I: Bond lengths in the optimized structures and corresponding vibrational frequencies of the normal modes of the HgX_2 compounds at selected level of theories (both from the literature and used in this work). In all cases, linear structures of HgX_2 have been found to be the most stable ones.

Method	R_{HgX} [Å]	ν_{sym} [cm^{-1}]	ν_{asym} [cm^{-1}]	ν_{bend} [cm^{-1}]
		$HgCl_2$		
PBE0/aug–cc–pVTZ–PP[a]	2.257	355.5	411.4	101.5
PBE0–SO/aug–cc–pVTZ–PP[a]	2.253	362.3	414.6	101.9
CCSD(T)/CBS(TQ)[b]	2.2509	363.0	417.0	102.2
CCSD(T)–CV/CBS(TQ)[b]	2.2450	367.0	420.3	104.2
CCSD(T)–CV–SR/CBS(TQ)[b]	2.2447	366.7	420.1	104.2
CASPT2(12,10)/ANO–RCC–VQZP[c]	2.230	373.8	430.6	106.8
Electron Diffraction[d]	2.240, 2.252, 2.275			
UV gas phase[e]		365,366		70
Raman and IR gas phase[f]		355,358	413	100
Raman and IR matrix[g]		358.4	407.5	107
		$HgBr_2$		
PBE0/aug–cc–pVTZ–PP[a]	2.392	218.9	289.6	69.0
PBE0–SO/aug–cc–pVTZ–PP[a]	2.389	224.6	295.4	65.7
PBE0/Def2QZVP[c]	2.392	218.8	288.3	68.6
CCSD/Def2QZVP[c]	2.382	228.2	297.2	70.1
CCSD(T)/CBS(TQ)[b]	2.3853	224.6	295.3	68.5
CCSD(T)–CV/CBS(TQ)[b]	2.3764	227.5	298.4	70.1
CCSD(T)–CV–SO/CBS(TQ)[b]	2.3770	226.9	297.8	69.6
CASPT2(12,10)/ANO–RCC–VTZP[c]	2.374	228.6	276.3	70.2
CASPT2(12,10)/ANO–RCC–VQZP[c]	2.363	239.9	303.8	71.5
Electron Diffraction[h]	2.374, 2.41, 2.378			
UV gas phase[i]		229,221	295	41,53
Raman and IR gas phase[f]		220,218,221.8	293	68
Raman and IR matrix[j]		225	294	73
		HgI_2		
PBE0/aug–cc–pVTZ–PP[a]	2.578	156.9	231.7	52.8
PBE0–SO/aug–cc–pVTZ–PP[a]	2.578	164.2	239.9	51.4
CCSD(T)/aug–cc–pVTZ–PP[a]	2.568	160.1	235.6	53.8
CASPT2(12,10)/ANO–RCC–VQZP[c]	2.527	174.9	255.7	56.8
Electron Diffraction[k]	2.554, 2.5587			
UV gas phase[l]		156	235	33,46
Raman and IR gas phase[m]		155,158.4	237	51
Raman and IR matrix[j]		163.5	237.5	63

[a] Ref.[1] [b] Ref.[2] [c] This work [d] Ref.[3–5] [e] Ref.[6,7] [f] Ref.[8–10] [g] Ref.[11,12] [h] Ref.[3,5,13] [i] Ref.[6,14] [j] Ref.[11,12,15] [k] Ref.[3,16] [m] Ref.[9,10,17,18] [n] Ref.[15] [l] Ref.[6,19]

TABLE S.II: Bond lengths in the optimized structures and corresponding vibrational frequencies of the normal modes of the HgXY compounds at selected level of theories (both from the literature and used in this work). In all cases, linear structures of HgXY have been found to be the most stable ones.

Method	R_{HgX} [Å]	R_{HgY} [Å]	ν_{sym} [cm^{-1}]	ν_{asym} [cm^{-1}]	ν_{bend} [cm^{-1}]
			HgBrCl		
CCSD(T)/CBS(TQ)[a]	2.3761	2.2603	257.7	390.3	85.7
CCSD(T)–CV/CBS(TQ)[a]	2.3674	2.2542	260.8	393.9	87.4
CCSD(T)–CV–SO/CBS(TQ)[a]	2.3682	2.2539	260.2	393.6	87.0
CCSD(T)–CV–SO–SR/CBS(TQ)[a]	2.3685	2.2535	260.1	393.4	87.0
CASPT2(12,10)/ANO–RCC–VQZP[b]	2.353	2.240	271.0	411.1	88.3
Raman and IR gas phase[c]			253	385	83
Raman and IR matrix[d]			255	387.5	89,91
			HgClI		
CASPT2(12,10)/ANO–RCC–VQZP[b]	2.251	2.507	211.8	394.3	80.1
Raman and IR gas phase[c]			196	371	74
Raman and IR matrix[d]			201.5	378.0	85,83.5
			HgBrI		
CASPT2(12,10)/ANO–RCC–VQZP[b]	2.374	2.515	187.9	285.8	62.9
Raman and IR gas phase[c]			182	266	60
Raman and IR matrix[d]			187.6	272.0	66

[a] Ref.[2]
[b] This work
[c] Ref.[9,10]
[d] Ref.[11,12]

S.II. ADDITIONAL TABLES

A. Allowed vertical electronic transitions of HgX_2 and HgXY

TABLE S.III: Symmetry–allowed vertical electronic transitions of $HgCl_2$ computed at the DKH3–SOC–MS–CASPT2(12,10)/ANO–RCC–VQZP level of theory at the ground–state equilibrium geometry, including vertical excitations energies in eV (ΔE) and oscillator strengths (f) for the spin–free (SF) and spin–orbit (SO) states (left and right parts, respectively), the main natural orbital excitations which characterize the SF states (columns 2 and 3, only weights larger than 10% are given, for more information see Table S.VIII), and the main SF states contributing to the SO states (columns 8 and 9, only weights larger than 2% are provided).

SF state	Weight [%]	Excitation	ΔE [eV]	f [au]	SO state/Ω state	Weight [%]	SF state	ΔE [eV]	f [au]
$1^1\Sigma_g^+$	92		0.00		$1^1\Sigma_{g0+}^+$ (1) 0_g^+	100	$1^1\Sigma_g^+$	0.00	
$1^3\Pi_u$	83	$\pi_u^{nb} \rightarrow \sigma_g^{+\star}$	5.85		$1^3\Pi_{u1}$ (1) 1_u	77	$1^3\Pi_u$	5.84	0.00517
						22	$1^1\Pi_u$		
					$1^3\Pi_{u0+}$ (1) 0_u^+	100	$1^3\Pi_u$	5.92	0.00001
$1^1\Pi_u$	84	$\pi_u^{nb} \rightarrow \sigma_g^{+\star}$	5.92	0.02415	$1^1\Pi_{u1}$ (2) 1_u	77	$1^1\Pi_u$	5.95	0.01880
						22	$1^3\Pi_u$		
$1^3\Sigma_u^+$	88	$\sigma_u^{+nb} \rightarrow \sigma_g^{+\star}$	6.22		$1^3\Sigma_{u1}^+$ (3) 1_u	99	$1^3\Sigma_u^+$	6.24	0.00020
$1^1\Sigma_u^+$	66	$\pi_g^{nb} \rightarrow \pi_u$	6.96	0.07999	$1^1\Sigma_{u0+}^+$ (2) 0_u^+	91	$1^1\Sigma_u^+$	6.95	0.06352
	22	$\sigma_u^{+nb} \rightarrow \sigma_g^{+\star}$				8	$1^3\Sigma_u^-$		
$2^3\Sigma_u^+$	88	$\pi_g^{nb} \rightarrow \pi_u$	7.02		$2^3\Sigma_{u1}^+$ (4) 1_u	74	$2^3\Sigma_u^+$	6.88	3.2E-06
						25	$1^3\Sigma_u^-$		
$1^3\Delta_u$	88	$\pi_g^{nb} \rightarrow \pi_u$	7.18		$1^3\Delta_{u1}$ (5) 1_u	100	$1^3\Delta_u$	7.02	0.00003
$1^3\Sigma_u^-$	88	$\pi_g^{nb} \rightarrow \pi_u$	7.32		$1^3\Sigma_{u0+}^-$ (3) 0_u^+	91	$1^3\Sigma_u^-$	7.36	0.02594
						8	$1^1\Sigma_u^+$		
					$1^3\Sigma_{u1}^-$ (6) 1_u	74	$1^3\Sigma_u^-$	7.49	6.3E-07
						26	$2^3\Sigma_u^+$		
$2^1\Sigma_u^+$	72	$\sigma_u^{+nb} \rightarrow \sigma_g^{+\star}$	8.61	2.03991	$2^1\Sigma_{u0+}^+$ (4) 0_u^+	50	$2^1\Sigma_u^+$	8.53	0.96067
	24	$\pi_g^{nb} \rightarrow \pi_u$				50	$2^3\Pi_u$		
					$3^1\Sigma_{u0+}^+$ (5) 0_u^+	50	$2^1\Sigma_u^+$	8.73	1.07039
						50	$2^3\Pi_u$		

TABLE S.IV: Symmetry–allowed vertical electronic transitions of HgI_2 computed at the DKH3–SOC–MS–CASPT2(12,10)/ANO–RCC–VQZP level of theory at the ground–state equilibrium geometry, including vertical excitations energies in eV (ΔE) and oscillator strengths (f) for the spin–free (SF) and spin–orbit (SO) states (left and right parts, respectively), the main natural orbital excitations which characterize the SF states (columns 2 and 3, only weights larger than 10% are given, for more information see Table S.IX), and the main SF states contributing to the SO states (columns 8 and 9, only weights larger than 2% are provided).

SF state	Weight [%]	Excitation	ΔE [eV]	f [au]	SO state/Ω state		Weight [%]	SF state	ΔE [eV]	f [au]
$1^1\Sigma_g^+$	93		0.00		$1^1\Sigma_{g0+}^+$	(1) 0_g^+	99	$1^1\Sigma_g^+$	0.00	
$1^3\Pi_u$	86	$\pi_u^{nb} \rightarrow \sigma_g^{+\star}$	4.53		$1^3\Pi_{u1}$	(1) 1_u	65	$1^3\Pi_u$	4.35	0.00440
							32	$1^1\Pi_u$		
					$1^3\Pi_{u0+}$	(1) 0_u^+	96	$1^3\Pi_u$	4.85	0.04102
							3	$1^1\Sigma_u^+$		
$1^1\Pi_u$	87	$\pi_u^{nb} \rightarrow \sigma_g^{+\star}$	4.65	0.01306	-[a]	(2) 1_u	48	$1^3\Sigma_u^+$	4.57	0.00416
							39	$1^1\Pi_u$		
							12	$1^3\Pi_u$		
$1^3\Sigma_u^+$	83	$\sigma_u^{+nb} \rightarrow \sigma_g^{+\star}$	4.87		-[a]	(3) 1_u	48	$1^3\Sigma_u^+$	5.29	0.00407
							27	$1^1\Pi_u$		
							19	$1^3\Pi_u$		
$1^1\Sigma_u^+$	66	$\pi_g^{nb} \rightarrow \pi_u$	5.73	0.08338	$1^1\Sigma_{u0+}^+$	(2) 0_u^+	94	$1^1\Sigma_u^+$	5.82	0.05127
	25	$\sigma_u^{+nb} \rightarrow \sigma_g^{+\star}$					4	$1^3\Pi_u$		
							2	$1^3\Sigma_u^-$		
$2^3\Sigma_u^+$	83	$\pi_g^{nb} \rightarrow \pi_u$	5.83		$2^3\Sigma_{u1}^+$	(4) 1_u	58	$2^3\Sigma_u^+$	5.48	0.00027
							35	$1^3\Sigma_u^-$		
							3	$1^3\Sigma_u^+$		
							3	$1^3\Pi_u$		
$1^3\Delta_u$	89	$\pi_g^{nb} \rightarrow \pi_u$	5.96		$1^3\Delta_{u1}$	(5) 1_u	100	$1^3\Delta_u$	6.06	0.00280
$1^3\Sigma_u^-$	89	$\pi_g^{nb} \rightarrow \pi_u$	6.09		$1^3\Sigma_{u0+}^-$	(3) 0_u^+	97	$1^3\Sigma_u^-$	6.14	0.00723
							2	$1^1\Sigma_u^+$		
					$1^3\Sigma_{u1}^-$	(6) 1_u	61	$1^3\Sigma_u^-$	6.57	0.00383
							37	$2^3\Sigma_u^+$		
$2^1\Sigma_u^+$	69	$\sigma_u^{+nb} \rightarrow \sigma_g^{+\star}$	7.35	3.18911	$2^1\Sigma_{u0+}^+$	(4) 0_u^+	100	$2^1\Sigma_u^+$	7.44	3.15275
	26	$\pi_g^{nb} \rightarrow \pi_u$								

[a] Strong mixing between $1^3\Sigma_u^+$ and $1^1\Pi_u$ (in favour for $1^3\Sigma_u^+$) prevents assigning the spatial symmetry of this SO state unambiguously.

TABLE S.V: Symmetry–allowed vertical electronic transitions of HgClI computed at the DKH3–SOC–MS–CASPT2(12,10)/ANO–RCC–VQZP level of theory at the ground–state equilibrium geometry, including vertical excitations energies in eV (ΔE) and oscillator strengths (f) for the spin–free (SF) and spin–orbit (SO) states (left and right parts, respectively), the corresponding SF states of $D_{\infty h}$ symmetry, the main natural orbital excitations which characterize the SF states (columns 3 and 4, only weights larger than 10% are given, for more information see Table S.XI), and the main SF states contributing to the SO states (columns 9 and 10, only weights larger than 2% are provided).

SF state	(D_{2h})	Weight [%]	Excitation	ΔE [eV]	f [au]	SO state/Ω state	Weight [%]	SF state	ΔE [eV]	f [au]
$1^1\Sigma^+$	($1^1\Sigma_g^+$)	95		0.00		$1^1\Sigma_{0+}^+$ (1) 0_+	100	$1^1\Sigma^+$	0.00	
$1^3\Pi$	($1^3\Pi_g$)	88	$\pi_2^{nb} \rightarrow \sigma^{+\star}$	4.45		$1^3\Pi_1$ (1) 1	76	$1^3\Pi$	4.33	0.00086
							23	$1^1\Pi$		
						$1^3\Pi_{0+}$ (2) 0_+	100	$1^3\Pi$	4.77	0.01033
$1^1\Pi$	($1^1\Pi_g$)	80	$\pi_2^{nb} \rightarrow \sigma^{+\star}$	4.76	0.00274	$1^1\Pi_1$ (2) 1	68	$1^1\Pi$	4.85	0.00174
							19	$1^3\Pi$		
							13	$1^3\Sigma^+$		
$1^3\Sigma^+$	($1^3\Sigma_u^+$)	69	$\sigma^{+nb} \rightarrow \sigma^{+\star}$	5.48		$1^3\Sigma_1^+$ (4) 1	61	$1^3\Sigma^+$	5.62	0.00022
		16	$\pi_2^{nb} \rightarrow \pi$				14	$2^3\Pi$		
							9	$2^1\Pi$		
							7	$1^1\Pi$		
							3	$2^3\Sigma^+$		
$2^3\Pi$	($1^3\Pi_u$)	87	$\pi_1^{nb} \rightarrow \sigma^{+\star}$	5.56		$2^3\Pi_1$ (3) 1	77	$2^3\Pi$	5.55	0.00036
							19	$1^3\Sigma^+$		
							2	$2^1\Pi$		
						$2^3\Pi_{0+}$ (3) 0_+	100	$2^3\Pi$	5.66	0.00307
$2^1\Pi$	($1^1\Pi_u$)	79	$\pi_1^{nb} \rightarrow \sigma^{+\star}$	5.82	0.01120	$2^1\Pi_1$ (5) 1	75	$2^1\Pi$	5.87	0.00871
							13	$2^3\Sigma^+$		
							8	$1^3\Sigma^-$		
$2^3\Sigma^+$	($2^3\Sigma_u^+$)	49	$\pi_2^{nb} \rightarrow \pi$	6.21		$2^3\Sigma_1^+$ (6) 1	49	$2^3\Sigma^+$	5.89	0.00152
		23	$\sigma^{+nb} \rightarrow \sigma^{+\star}$				25	$1^3\Sigma^-$		
		18	$\pi_1^{nb} \rightarrow \pi$				13	$2^1\Pi$		
							5	$2^3\Pi$		
							5	$1^3\Sigma^+$		
$2^1\Sigma^+$	($1^1\Sigma_u^+$)	59	$\pi_2^{nb} \rightarrow \pi$	6.28	0.03850	$2^1\Sigma_{0+}^+$ (4) 0_+	97	$2^1\Sigma^+$	6.31	0.02758
		20	$\sigma^{+nb} \rightarrow \sigma^{+\star}$				2	$3^3\Pi$		
$1^3\Delta$	($1^3\Delta_u$)	88	$\pi_2^{nb} \rightarrow \pi$	6.36		$1^3\Delta_1$ (7) 1	94	$1^3\Delta$	6.38	0.00449
							3	$3^3\Pi$		
							2	$3^1\Pi$		
$1^3\Sigma^-$	($1^3\Sigma_u^-$)	88	$\pi_2^{nb} \rightarrow \pi$	6.53		$1^3\Sigma_{0+}^-$ (5) 0_+	96	$1^3\Sigma^-$	6.53	0.00005
							4	$3^3\Pi$		
						$1^3\Sigma_1^-$ (8) 1	39	$1^3\Sigma^-$	6.85	0.00248
							34	$3^3\Sigma^+$		
							21	$2^3\Sigma^+$		
							3	$3^1\Pi$		

Table continued on next page

TABLE S.V: Continue...

SF state	(D_{2h})	Weight [%]	Excitation	ΔE [eV]	f [au]	SO state/Ω state	Weight [%]	SF state	ΔE [eV]	f [au]
$3^3\Sigma^+$	($1^3\Sigma_g^+$)	41	$\pi_1^{nb} \rightarrow \pi$	6.89		$3^3\Sigma_1^+$ (9) 1	60	$3^3\Sigma^+$	6.94	0.00172
		26	$\sigma_1^+ \rightarrow \sigma^{+\star}$				22	$1^3\Sigma^-$		
		23	$\pi_2^{nb} \rightarrow \pi$				11	$2^3\Sigma^+$		
							3	$3^3\Pi$		
							2	$2^3\Sigma^-$		
$3^1\Sigma^+$	($2^1\Sigma_g^+$)	57	$\pi_1^{nb} \rightarrow \pi$	7.34	0.31756	$3^1\Sigma_{0+}^+$ (6) 0_+	83	$3^1\Sigma^+$	7.33	0.21391
		19	$\sigma_1^+ \rightarrow \sigma^{+\star}$				11	$2^3\Sigma^-$		
							6	$3^3\Pi$		
$2^3\Delta$	($1^3\Delta_g$)	85	$\pi_1^{nb} \rightarrow \pi$	7.46		$2^3\Delta_1$ (10) 1	71	$2^3\Delta$	7.30	0.00100
							15	$4^3\Sigma^+$		
							8	$2^3\Sigma^-$		
							3	$3^3\Pi$		
$4^3\Sigma^+$	($2^3\Sigma_g^+$)	61	$\sigma_1^+ \rightarrow \sigma^{+\star}$	7.48		$4^3\Sigma_1^+$ (11) 1	45	$4^3\Sigma^+$	7.31	0.00023
		25	$\pi_1^{nb} \rightarrow \pi$				26	$2^3\Sigma^-$		
							25	$2^3\Delta$		
							2	$3^3\Sigma^+$		
$2^3\Sigma^-$	($1^3\Sigma_g^-$)	85	$\pi_1^{nb} \rightarrow \pi$	7.60		$2^3\Sigma_1^-$ (8) 0_+	73	$2^3\Sigma^-$	7.66	0.61485
							15	$4^1\Sigma^+$		
							10	$3^1\Sigma^+$		
$3^3\Pi$	($2^3\Pi_u$)	52	$\sigma_1^+ \rightarrow \pi$	7.71		$3^3\Pi_1$ (12) 1	55	$3^3\Pi$	7.67	0.01509
		40	$\sigma^{+nb} \rightarrow \pi$				33	$3^1\Pi$		
							6	$1^3\Delta$		
							4	$2^3\Delta$		
						$3^3\Pi_{0+}$ (7) 0_+	84	$3^3\Pi$	7.61	0.03067
							6	$3^1\Sigma^+$		
							4	$4^1\Sigma^+$		
							4	$1^3\Sigma^-$		
$4^1\Sigma^+$	($3^1\Sigma_g^+$)	41	$\sigma_1^+ \rightarrow \sigma^{+\star}$	7.72	1.86775	$4^1\Sigma_{0+}^+$ (9) 0_+	80	$4^1\Sigma^+$	7.81	1.32056
		25	$\sigma^{+nb} \rightarrow \sigma^{+\star}$				14	$2^3\Sigma^-$		
		11	$\pi_1^{nb} \rightarrow \pi$				4	$3^3\Pi$		

TABLE S.VI: Symmetry–allowed vertical electronic transitions of HgBrI computed at the DKH3–SOC–MS–CASPT2(12,10)/ANO–RCC–VQZP level of theory at the ground–state equilibrium geometry, including vertical excitations energies in eV (ΔE) and oscillator strengths (f) for the spin–free (SF) and spin–orbit (SO) states (left and right parts, respectively), the corresponding SF states of $D_{\infty h}$ symmetry, the main natural orbital excitations which characterize the SF states (columns 3 and 4, only weights larger than 10% are given, for more information see Table S.XII), and the main SF states contributing to the SO states (columns 9 and 10, only weights larger than 2% are provided).

SF state	(D_{2h})	Weight [%]	Excitation	ΔE [eV]	f [au]	SO state/Ω state	Weight [%]	SF state	ΔE [eV]	f [au]
$1^1\Sigma^+$	($1^1\Sigma_g^+$)	92		0.00		$1^1\Sigma_{0+}^+$ (1) 0_+	99	$1^1\Sigma^+$	0.00	
$1^3\Pi$	($1^3\Pi_g$)	88	$\pi_2^{nb} \rightarrow \sigma^{+\star}$	4.27		$1^3\Pi_1$ (1) 1	65	$1^3\Pi$	4.10	0.00073
							34	$1^1\Pi$		
						$1^3\Pi_{0+}$ (2) 0_+	100	$1^3\Pi$	4.57	0.00471
$1^1\Pi$	($1^1\Pi_g$)	86	$\pi_2^{nb} \rightarrow \sigma^{+\star}$	4.44	0.00151	$1^1\Pi_1$ (2) 1	58	$1^1\Pi$	4.60	0.00121
							29	$1^3\Pi$		
							11	$1^3\Sigma^+$		
$2^3\Pi$	($1^3\Pi_u$)	86	$\pi_1^{nb} \rightarrow \sigma^{+\star}$	4.98		$2^3\Pi_1$ (3) 1	71	$2^3\Pi$	4.88	0.00462
							25	$2^1\Pi$		
							3	$1^3\Sigma^+$		
						$2^3\Pi_{0+}$ (3) 0_+	100	$2^3\Pi$	5.19	0.01382
$2^1\Pi$	($1^1\Pi_u$)	85	$\pi_1^{nb} \rightarrow \sigma^{+\star}$	5.10	0.01888	$2^1\Pi_1$ (4) 1	47	$2^1\Pi$	5.06	0.00687
							39	$1^3\Sigma^+$		
							8	$2^3\Pi$		
							4	$1^1\Pi$		
							2	$1^3\Pi$		
$1^3\Sigma^+$	($1^3\Sigma_u^+$)	77	$\sigma^{+nb} \rightarrow \sigma^{+\star}$	5.15		$1^3\Sigma_1^+$ (5) 1	46	$1^3\Sigma^+$	5.45	0.00672
							28	$2^1\Pi$		
							19	$2^3\Pi$		
							3	$1^1\Pi$		
							2	$1^3\Pi$		
$2^1\Sigma^+$	($1^1\Sigma_u^+$)	65	$\pi_2^{nb} \rightarrow \pi$	6.04	0.07532	$2^1\Sigma_{0+}^+$ (4) 0_+	97	$2^1\Sigma^+$	6.08	0.05780
		20	$\sigma^{+nb} \rightarrow \sigma^{+\star}$							
$2^3\Sigma^+$	($2^3\Sigma_u^+$)	72	$\pi_2^{nb} \rightarrow \pi$	6.09		$2^3\Sigma_1^+$ (6) 1	64	$2^3\Sigma^+$	5.77	0.00002
							34	$1^3\Sigma^-$		
$1^3\Delta$	($1^3\Delta_u$)	86	$\pi_2^{nb} \rightarrow \pi$	6.24		$1^3\Delta_1$ (7) 1	94	$1^3\Delta$	6.28	0.00264
							2	$3^3\Pi$		
							2	$3^1\Pi$		
$1^3\Sigma^-$	($1^3\Sigma_u^-$)	87	$\pi_2^{nb} \rightarrow \pi$	6.40		$1^3\Sigma_{0+}^-$ (5) 0_+	96	$1^3\Sigma^-$	6.41	0.00099
							3	$3^3\Pi$		
						$1^3\Sigma_1^-$ (9) 1	58	$1^3\Sigma^-$	6.76	0.00315
							32	$2^3\Sigma^+$		
							3	$3^3\Sigma^+$		
							3	$3^1\Pi$		

Table continued on next page

TABLE S.VI: Continue...

SF state	(D_{2h})	Weight [%]	Excitation	ΔE [eV]	f [au]	SO state/Ω state	Weight [%]	SF state	ΔE [eV]	f [au]
$3^3\Sigma^+$	($1^3\Sigma_g^+$)	67	$\pi_1^{nb} \rightarrow \pi$	6.58		$3^3\Sigma_1^+$ (8) 1	74	$3^3\Sigma^+$	6.46	2.5E-06
		12	$\sigma_1^+ \rightarrow \sigma^{+\star}$				20	$2^3\Sigma^-$		
							3	$4^3\Sigma^+$		
$2^3\Delta$	($1^3\Delta_g$)	87	$\pi_1^{nb} \rightarrow \pi$	6.91		$2^3\Delta_1$ (10) 1	76	$2^3\Delta$	6.81	0.00004
							9	$3^3\Pi$		
							6	$3^1\Pi$		
							4	$4^3\Sigma^+$		
$3^1\Sigma^+$	($2^1\Sigma_g^+$)	69	$\pi_1^{nb} \rightarrow \pi$	7.02	0.13343	$3^1\Sigma_{0+}^+$ (6) 0_+	52	$3^1\Sigma^+$	6.97	0.05845
		10	$\sigma_1^+ \rightarrow \sigma^{+\star}$				26	$2^3\Sigma^-$		
							21	$3^3\Pi$		
$4^3\Sigma^+$	($2^3\Sigma_g^+$)	69	$\sigma_1^+ \rightarrow \sigma^{+\star}$	7.05		$4^3\Sigma_1^+$ (11) 1	52	$4^3\Sigma^+$	6.95	0.00027
		14	$\pi_1^{nb} \rightarrow \pi$				18	$2^3\Sigma^-$		
							16	$3^3\Sigma^+$		
							9	$2^3\Delta$		
$2^3\Sigma^-$	($1^3\Sigma_g^-$)	86	$\pi_1^{nb} \rightarrow \pi$	7.09		$2^3\Sigma_1^-$ (7) 0_+	54	$2^3\Sigma^-$	7.12	0.09376
							41	$3^1\Sigma^+$		
							4	$3^3\Pi$		
$3^3\Pi$	($2^3\Pi_g$)	82	$\sigma^{+nb} \rightarrow \pi$	7.39		$3^3\Pi_1$ (12) 1	34	$3^3\Pi$	7.34	0.00003
							38	$2^3\Sigma^-$		
							16	$4^3\Sigma^+$		
							6	$3^3\Sigma^+$		
							2	$2^3\Delta$		
						$3^3\Pi_{0+}$ (8) 0_+	70	$3^3\Pi$	7.38	0.01211
							19	$2^3\Sigma^-$		
							6	$3^1\Sigma^+$		
							2	$1^3\Sigma^-$		
$4^1\Sigma^+$	($3^1\Sigma_g^+$)	37	$\sigma_1^+ \rightarrow \sigma^{+\star}$	7.61	2.57561	$4^1\Sigma_{0+}^+$ (9) 0_+	98	$4^1\Sigma^+$	7.67	2.53150
		29	$\sigma^{+nb} \rightarrow \sigma^{+\star}$							
		20	$\pi_2^{nb} \rightarrow \pi$							

B. Multiconfigurational nature of the spin–free states of HgX_2 and HgXY

TABLE S.VII: Main electronic configurations of the most relevant low–lying electronic SF states in the UV–Vis spectroscopy of $HgCl_2$ determined with the DKH3–CASSCF(12,10)/ANO–RCC–VQZP methodology at the DKH3–CASPT2(12,10)/ANO–RCC–VQZP optimized geometry. Only configuration of weights larger than 2% are given.

SF state	Configuration	Weight [%]
$1^1\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{0}\ \sigma_u^{+\,0}$	92.5
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	2.3
$1^1\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	66.4
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	21.7
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.5
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.5
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	2.2
$2^1\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	72.4
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	24.2
$1^1\Pi_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	84.3
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	6.1
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{0}\ \sigma_u^{+\,1}$	3.2
$1^1\Sigma_u^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	87.9
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.7
$1^1\Delta_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	88.3
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.1
$1^3\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	87.8
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	4.6
$2^3\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	87.7
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.5
$1^3\Pi_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	83.0
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	4.3
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{0}\ \sigma_u^{+\,1}$	3.9
$1^3\Sigma_u^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	87.7
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.5
$1^3\Delta_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	87.7
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.5

SF state	Configuration	Weight [%]
$1^1\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{0}\ \sigma_u^{+\,0}$	92.5
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	2.3
$2^1\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	55.9
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	30.7
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,0}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	3.1
$1^1\Pi_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	85.1
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	4.1
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.0
$1^1\Sigma_g^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	87.1
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	5.8
$1^1\Delta_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	86.8
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	5.8
$1^3\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	54.6
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	32.9
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.7
$2^3\Sigma_g^+$	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	55.5
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	32.0
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	2.9
$1^3\Pi_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	87.6
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	2.7
$1^3\Sigma_g^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	85.4
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	6.8
$1^3\Delta_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	85.8
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	6.8

TABLE S.VIII: Main electronic configurations of the most relevant low–lying electronic SF states in the UV–Vis spectroscopy of $HgBr_2$ determined with the DKH3–CASSCF(12,10)/ANO–RCC–VQZP methodology at the DKH3–CASPT2(12,10)/ANO–RCC–VQZP optimized geometry. Only configuration of weights larger than 2% are given.

SF state	Configuration	Weight [%]
$1^1\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{0}\ \sigma_u^{+\,0}$	92.8
$1^1\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	65.1
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	23.4
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.6
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	2.8
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	2.2
$2^1\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	70.5
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	25.8
$1^1\Pi_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	85.6
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	6.1
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{0}\ \sigma_u^{+\,1}$	2.6
$1^1\Sigma_u^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	88.2
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.6
$1^1\Delta_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	88.6
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.1
$1^3\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	87.7
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	4.2
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	2.5
$2^3\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	87.1
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.5
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	2.3
$1^3\Pi_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	84.5
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	4.2
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{0}\ \sigma_u^{+\,1}$	3.3
$1^3\Sigma_u^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	88.0
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.5
$1^3\Delta_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	89.3
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.4

SF state	Configuration	Weight [%]
$1^1\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{0}\ \sigma_u^{+\,0}$	92.8
$2^1\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	63.5
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	22.8
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,0}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	2.7
$1^1\Pi_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	85.6
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	4.2
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.8
$1^1\Sigma_g^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	87.9
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	5.3
$1^1\Delta_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	87.6
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	5.3
$1^3\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	68.5
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	19.1
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	5.3
$2^3\Sigma_g^+$	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	68.2
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	18.8
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.5
$1^3\Pi_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	88.0
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	2.6
$1^3\Sigma_g^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	86.1
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	6.4
$1^3\Delta_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	86.6
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	6.5

TABLE S.IX: Main electronic configurations of the most relevant low–lying electronic SF states in the UV–Vis spectroscopy of HgI_2 determined with the DKH3–CASSCF(12,10)/ANO–RCC–VQZP methodology at the DKH3–CASPT2(12,10)/ANO–RCC–VQZP optimized geometry. Only configuration of weights larger than 2% are given.

SF state	Configuration	Weight [%]
$1^1\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{0}\ \sigma_u^{+\,0}$	93.0
$1^1\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	65.6
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	24.7
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	2.9
$2^1\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	68.8
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	25.8
$1^1\Pi_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	87.0
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	5.7
$1^1\Sigma_u^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	88.9
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.2
$1^1\Delta_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	89.0
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.2
$1^3\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	83.1
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	3.4
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	7.8
$2^3\Sigma_u^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	82.5
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.8
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	7.5
$1^3\Pi_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	86.3
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	3.7
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{0}\ \sigma_u^{+\,1}$	2.4
$1^3\Sigma_u^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	89.0
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.9
$1^3\Delta_u$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	89.1
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.0

SF state	Configuration	Weight [%]
$1^1\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{0}\ \sigma_u^{+\,0}$	93.0
$2^1\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	72.6
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	14.0
$1^1\Pi_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	86.4
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	3.9
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	3.6
$1^1\Sigma_g^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	89.2
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.3
$1^1\Delta_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	89.0
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.4
$1^3\Sigma_g^+$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	82.0
	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	6.5
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	5.1
$2^3\Sigma_g^+$	$\sigma_g^{+\,1}\ \pi_u^{nb\,4}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	78.7
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	6.4
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	4.1
$1^3\Pi_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,1}\ \pi_u^{0}\ \sigma_u^{+\,0}$	88.2
	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,2}\ \pi_u^{0}\ \sigma_u^{+\,0}$	2.1
$1^3\Sigma_g^-$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	87.5
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	5.5
$1^3\Delta_g$	$\sigma_g^{+\,2}\ \pi_u^{nb\,3}\ \pi_g^{nb\,4}\ \sigma_u^{+nb\,2}\ \sigma_g^{+\star\,0}\ \pi_u^{1}\ \sigma_u^{+\,0}$	87.9
	$\sigma_g^{+\,2}\ \pi_u^{nb\,4}\ \pi_g^{nb\,3}\ \sigma_u^{+nb\,1}\ \sigma_g^{+\star\,1}\ \pi_u^{1}\ \sigma_u^{+\,0}$	5.5

TABLE S.X: Main electronic configurations of the most relevant low–lying electronic SF states in the UV–Vis spectroscopy of HgBrCl determined with the DKH3–CASSCF(12,10)/ANO–RCC–VQZP methodology at the DKH3–CASPT2(12,10)/ANO–RCC–VQZP optimized geometry. Only configuration of weights larger than 2% are given.

SF state	Configuration	Weight [%]
$1^1\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{0}\ \sigma_2^{+\,0}$	94.6
$2^1\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	62.7
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	23.2
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	3.6
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	2.7
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	2.2
$3^1\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	54.7
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	27.9
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,0}\ \sigma^{+\star\,2}\ \pi^{0}\ \sigma_2^{+\,0}$	3.0
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	3.0
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	2.0
$4^1\Sigma^+$	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	50.0
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	26.2
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	4.2
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,0}\ \sigma^{+\star\,2}\ \pi^{0}\ \sigma_2^{+\,0}$	3.7
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	3.6
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{0}\ \sigma_2^{+\,0}$	2.5
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	2.0
$1^1\Pi$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	84.3
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	3.4
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	2.7
$2^1\Pi$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	82.5
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,2}\ \pi^{0}\ \sigma_2^{+\,0}$	4.2
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	3.3
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,2}\ \pi^{0}\ \sigma_2^{+\,0}$	2.1
$1^1\Sigma^-$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	88.6
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	2.7
$2^1\Sigma^-$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	88.5
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	3.9
$1^1\Delta$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	88.8
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	2.7
$2^1\Delta$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	88.0
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	3.8
$1^3\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	85.5
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	3.9
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,2}\ \pi^{0}\ \sigma_2^{+\,0}$	2.3
$2^3\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	72.3
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	11.1
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	5.4
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	2.1
$3^3\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	38.4
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	37.7
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	12.9
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	2.6
$4^3\Sigma^+$	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	48.6
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	38.2
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	3.0
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	2.1
$1^3\Pi$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	85.8
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	3.4
$2^3\Pi$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	83.4
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{0}\ \sigma_2^{+\,0}$	3.5
$3^3\Pi$	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	62.5
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	28.6
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	2.9
$1^3\Sigma^-$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	79.6
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	10.3
$2^3\Sigma^-$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	76.1
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	10.5
	$\sigma_1^{+\,1}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	3.8
$1^3\Delta$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	80.1
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	9.9
$2^3\Delta$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	77.0
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^{1}\ \sigma_2^{+\,0}$	10.2
	$\sigma_1^{+\,1}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^{1}\ \sigma_2^{+\,0}$	3.9

TABLE S.XI: Main electronic configurations of the most relevant low–lying electronic SF states in the UV–Vis spectroscopy of HgClI determined with the DKH3–CASSCF(12,10)/ANO–RCC–VQZP methodology at the DKH3–CASPT2(12,10)/ANO–RCC–VQZP optimized geometry. Only configuration of weights larger than 2% are given.

SF state	Configuration	Weight [%]
$1^1\Sigma^+$	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^0\sigma_2^{+\,0}$	94.5
$2^1\Sigma^+$	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	59.3
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	20.5
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	7.9
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	3.4
	$\sigma_1^{+\,1}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	2.7
$3^1\Sigma^+$	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	57.3
	$\sigma_1^{+\,1}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	19.1
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	5.6
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	6.2
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,0}\,\sigma^{+\star\,2}\,\pi^0\sigma_2^{+\,0}$	2.2
$4^1\Sigma^+$	$\sigma_1^{+\,1}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	41.0
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	25.0
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	10.7
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	9.4
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,0}\,\sigma^{+\star\,2}\,\pi^0\sigma_2^{+\,0}$	3.1
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.4
$1^1\Pi$	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	80.4
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	7.3
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,2}\,\pi^0\sigma_2^{+\,0}$	2.6
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.4
$2^1\Pi$	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	79.0
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	7.3
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,1}\,\sigma^{+\star\,2}\,\pi^0\sigma_2^{+\,0}$	2.9
	$\sigma_1^{+\,1}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,2}\,\pi^0\sigma_2^{+\,0}$	2.3
	$\sigma_1^{+\,1}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,2}\,\pi^0\sigma_2^{+\,0}$	2.3
$3^1\Pi$	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	58.6
	$\sigma_1^{+\,1}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	30.8
	$\sigma_1^{+\,1}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	6.1
$1^1\Sigma^-$	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	86.7
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.7
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.5
$2^1\Sigma^-$	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	87.0
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	3.1
$1^1\Delta$	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	87.0
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.7
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.5
$2^1\Delta$	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	87.0
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	3.1
$1^3\Sigma^+$	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	68.9
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	15.6
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	6.1
$2^3\Sigma^+$	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	49.3
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	22.8
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	17.5
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.7
$3^3\Sigma^+$	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	40.6
	$\sigma_1^{+\,1}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	26.1
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	23.0
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.5
$4^3\Sigma^+$	$\sigma_1^{+\,1}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	60.6
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	24.8
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	3.0
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.3
$1^3\Pi$	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	87.9
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,1}\,\sigma^{+\star\,2}\,\pi^0\sigma_2^{+\,0}$	2.2
$2^3\Pi$	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^0\sigma_2^{+\,0}$	87.4
$3^3\Pi$	$\sigma_1^{+\,1}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	51.9
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	39.5
	$\sigma_1^{+\,1}\,\pi_1^{nb\,4}\,\pi_2^{nb\,4}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.6
$1^3\Sigma^-$	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	87.7
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.6
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	2.6
$2^3\Sigma^-$	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	84.6
	$\sigma_1^{+\,1}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	4.0
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	2.5
$1^3\Delta$	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	88.2
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,1}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	2.7
	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	2.1
$2^3\Delta$	$\sigma_1^{+\,2}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	85.4
	$\sigma_1^{+\,1}\,\pi_1^{nb\,3}\,\pi_2^{nb\,4}\,\sigma^{+nb\,2}\,\sigma^{+\star\,1}\,\pi^1\sigma_2^{+\,0}$	4.1
	$\sigma_1^{+\,2}\,\pi_1^{nb\,4}\,\pi_2^{nb\,3}\,\sigma^{+nb\,2}\,\sigma^{+\star\,0}\,\pi^1\sigma_2^{+\,0}$	2.1

TABLE S.XII: Main electronic configurations of the most relevant low–lying electronic SF states in the UV–Vis spectroscopy of HgBrI determined with the DKH3–CASSCF(12,10)/ANO–RCC–VQZP methodology at the DKH3–CASPT2(12,10)/ANO–RCC–VQZP optimized geometry. Only configuration of weights larger than 2% are given.

SF state	Configuration	Weight [%]
$1^1\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^0\ \sigma_2^{+\,0}$	91.7
$2^2\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	65.1
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	19.6
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	4.1
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	3.2
$3^1\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	69.1
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	10.3
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	6.4
$4^1\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	29.3
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	36.8
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	19.9
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,2}\ \pi^0\ \sigma_2^{+\,0}$	2.7
$1^1\Pi$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	86.0
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,2}\ \pi^0\ \sigma_2^{+\,0}$	3.7
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	2.8
$2^1\Pi$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	84.7
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,2}\ \pi^0\ \sigma_2^{+\,0}$	5.7
$1^1\Sigma^-$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	87.8
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	3.0
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	2.7
$2^1\Sigma^-$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	88.7
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	4.4
$1^1\Delta$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	87.9
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	3.0
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	2.6
$2^1\Delta$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	88.5
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	4.4

SF state	Configuration	Weight [%]
$1^3\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	76.9
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	8.2
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,2}\ \pi^0\ \sigma_2^{+\,0}$	3.9
$2^3\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	71.8
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	3.8
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	9.4
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	2.3
$3^3\Sigma^+$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	66.7
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	9.5
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	12.1
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	2.8
$4^3\Sigma^+$	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	69.1
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	13.5
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	2.9
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	3.5
	$\sigma_1^{+\,1}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	3.1
$1^3\Pi$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	88.1
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,2}\ \pi^0\ \sigma_2^{+\,0}$	2.2
$2^3\Pi$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^0\ \sigma_2^{+\,0}$	85.7
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,2}\ \pi^0\ \sigma_2^{+\,0}$	3.0
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^0\ \sigma_2^{+\,1}$	2.2
$3^3\Pi$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	82.3
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	9.3
	$\sigma_1^{+\,1}\ \pi_1^{nb\,4}\ \pi_2^{nb\,4}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	3.5
$1^3\Sigma^-$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	86.8
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	3.0
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	3.4
$2^3\Sigma^-$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	86.5
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	4.2
	$\sigma_1^{+\,1}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	2.1
$1^3\Delta$	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	86.4
	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	3.4
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	3.2
$2^3\Delta$	$\sigma_1^{+\,2}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,0}\ \pi^1\ \sigma_2^{+\,0}$	86.5
	$\sigma_1^{+\,2}\ \pi_1^{nb\,4}\ \pi_2^{nb\,3}\ \sigma^{+nb\,1}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	4.1
	$\sigma_1^{+\,1}\ \pi_1^{nb\,3}\ \pi_2^{nb\,4}\ \sigma^{+nb\,2}\ \sigma^{+\star\,1}\ \pi^1\ \sigma_2^{+\,0}$	2.1

C. Extended data on the energetics of the excited states of HgX_2 and HgXY

TABLE S.XIII: Main vertical excitation energies (ΔE) in eV and associated oscillator strength (f) values obtained for symmetrical HgX_2 compounds from the computations of the SF states (SOC not considered) with the DKH3–MS–CASPT2(12,10)/ANO–RCC–VQZP methodology at equilibrium geometries (see computational details in Section II.A). Energetic ordering of states corresponds to the one of $HgBr_2$.

	$HgCl_2$		$HgBr_2$		HgI_2	
SF state	ΔE [eV]	f [au]	ΔE [eV]	f [au]	ΔE [eV]	f [au]
$1^1\Sigma_g^+$	0.00		0.00		0.00	
$1^3\Pi_g$	5.15		4.57		4.04	
$1^1\Pi_g$	5.23		4.72		4.17	
$1^3\Pi_u$	5.85		5.17		4.53	
$1^1\Pi_u$	5.92	0.02415	5.29	0.02444	4.65	0.01306
$1^3\Sigma_u^+$	6.22		5.5		4.87	
$1^1\Sigma_u^+$	6.96	0.07999	6.36	0.09646	5.73	0.08338
$2^3\Sigma_u^+$	7.02		6.45		5.83	
$1^3\Delta_u$	7.18		6.59		5.96	
$1^1\Delta_u$	7.20		6.62		5.96	
$1^1\Sigma_u^-$	7.25		6.67		6.01	
$1^3\Sigma_g^+$	7.00		6.71		6.12	
$1^3\Sigma_u^-$	7.32		6.74		6.09	
$1^3\Delta_g$	7.86		7.15		6.41	
$2^1\Sigma_g^+$	7.59		7.18		6.66	
$2^3\Sigma_g^+$	7.86		7.22		6.80	
$1^1\Delta_g$	7.94		7.25		6.54	
$1^1\Sigma_g^-$	7.99		7.29		6.52	
$1^3\Sigma_g^-$	8.05		7.34		6.57	
$2^3\Pi_g$	8.59		7.87		7.03	
$2^1\Pi_g$	8.58		7.88		7.09	
$3^1\Sigma_g^+$	8.55		8.08		7.61	
$2^1\Sigma_u^+$	8.61	2.03991	8.08	2.52704	7.35	3.18911

TABLE S.XIV: Main vertical excitation energies (ΔE) in eV and associated oscillator strength (f) values obtained for mixed HgXY compounds from the computations of the SF states (SOC not considered) with the DKH3–MS–CASPT2(12,10)/ANO–RCC–VQZP methodology at equilibrium geometries (see computational details in Section II.A). Energetic ordering of states corresponds to the one of HgBrCl.

	HgBrCl		HgClI		HgBrI	
SF state	ΔE [eV]	f [au]	ΔE [eV]	f [au]	ΔE [eV]	f [au]
$1^1\Sigma^+$	0.00		0.00		0.00	
$1^3\Pi$	4.86		4.45		4.27	
$1^1\Pi$	5.15	0.00318	4.76	0.00274	4.44	0.00151
$2^3\Pi$	5.70		5.56		4.98	
$1^3\Sigma^+$	5.84		5.48		5.15	
$2^1\Pi$	6.00	0.01676	5.82	0.01120	5.10	0.01888
$2^3\Sigma^+$	6.66		6.21		6.09	
$2^1\Sigma^+$	6.66	0.05102	6.28	0.03850	6.04	0.07532
$1^3\Delta$	6.80		6.36		6.24	
$1^1\Delta$	6.85		6.44		6.26	
$1^1\Sigma^-$	6.92		6.45		6.32	
$3^3\Sigma^+$	6.95		6.89		6.58	
$1^3\Sigma^-$	6.99		6.53		6.40	
$3^1\Sigma^+$	7.51	0.00683	7.34	0.31756	7.02	0.13343
$2^3\Delta$	7.62		7.46		6.91	
$4^3\Sigma^+$	7.64		7.48		7.05	
$2^1\Delta$	7.72		7.53		6.98	
$2^1\Sigma^-$	7.76		7.54		7.03	
$2^3\Sigma^-$	7.81		7.60		7.09	
$4^1\Sigma^+$	8.14	1.54965	7.72	1.86775	7.61	2.57561
$3^3\Pi$	8.18		7.71		7.39	

TABLE S.XV: Main vertical excitation energies (ΔE) in eV and associated oscillator strength (f) values obtained for symmetrical HgX_2 compounds from the computations of the SO states with the DKH3–SOC–MS–CASPT2(12,10)/ANO–RCC–VQZP methodology at equilibrium geometries (see computational details in Section II.A).

	$HgCl_2$		$HgBr_2$		HgI_2	
SO state	ΔE [eV]	f [au]	ΔE [eV]	f [au]	ΔE [eV]	f [au]
(1) 0_g^+	0.00		0.00		0.00	
(1) 2_g	5.12		4.43		3.79	
(1) 1_g	5.14		4.49		3.85	
(1) 0_g^-	5.21		4.74		4.39	
(2) 0_g^+	5.21		4.75		4.42	
(2) 1_g	5.26		4.83		4.45	
(1) 2_u	5.81		5.04		4.30	
(1) 1_u	5.84	0.00517	5.09	0.00663	4.35	0.00440
(1) 0_u^-	5.91		5.26		4.53	
(2) 1_u	5.95	0.01880	5.32	0.01296	4.57	0.00416
(1) 0_u^+	5.92	0.00001	5.34	0.00645	4.85	0.04102
(2) 0_u^-	6.24		5.60		5.27	
(3) 1_u	6.24	0.00020	5.62	0.00474	5.29	0.00407
(4) 1_u	6.88	3.2E-06	6.21	1.9E-06	5.48	0.00027
(2) 2_u	6.94		6.25		5.47	
(2) 0_u^+	6.95	0.06352	6.39	0.09004	5.82	0.05127
(3) 0_u^-	6.95		6.45		5.87	
(5) 1_u	7.02	0.00003	6.53	0.00053	6.06	0.00280
(3) 1_g	7.00		6.65		5.87	
(1) 3_u	7.36		6.69		5.96	
(4) 0_u^-	7.35		6.71		6.07	
(2) 0_g^-	7.01		6.73		6.14	
(3) 0_u^+	7.36	0.02594	6.77	0.00389	6.14	0.00723
(2) 2_g	7.65		6.85		6.00	
(3) 2_u	7.44		6.98		6.52	
(6) 1_u	7.49	6.3E-07	7.03	0.00084	6.57	0.00383
(4) 1_g	7.72		7.05		6.30	
(5) 1_g	7.73		7.09		6.69	
(3) 0_g^+	7.59		7.18		6.49	
(3) 0_g^-	7.80		7.19		6.44	
(1) 3_g	8.03		7.24		6.41	
(4) 0_g^-	8.09		7.33		6.81	
(4) 0_g^+	8.04		7.37		6.68	
(3) 2_g	8.16		7.55		6.79	
(6) 1_g	8.23		7.60		6.91	
(5) 0_g^+	8.41		7.74		7.13	
(7) 1_g	8.41		7.74		7.17	
(5) 0_g^-	8.43		7.75		7.19	
(4) 0_u^+ [a]	8.53	0.96067	8.10	2.40671	7.44	3.15275

[a] Characterize with almost identical weights of the same SF states as state (5) 0_u^+ (ΔE = 8.73 eV, f=1.07039)

TABLE S.XVI: Main vertical excitation energies (ΔE) in eV and associated oscillator strength (f) values, obtained for asymmetrical HgXY compounds from the computations of the SO states with the DKH3–SOC–MS–CASPT2(12,10)/ANO–RCC–VQZP methodology at equilibrium geometries. Additionally, dipole moments of SO states (μ_z) in Debyes are reported (for orientation X–Hg–Y; positive end towards the second halogen Y).

	Cl–Hg–Br			Cl–Hg–I			Br–Hg–I		
SO state	ΔE [eV]	f [au]	μ_z [D]	ΔE [eV]	f [au]	μ_z [D]	ΔE [eV]	f [au]	μ_z [D]
(1) 0_+	0.00		0.65	0.00		1.07	0.00		0.38
(1) 2	4.75		3.84	4.21		4.85	4.03		4.02
(1) 1	4.83	0.00053	3.69	4.33	0.00086	4.91	4.10	0.00073	4.23
(1) 0_-	5.00		2.96	4.68		4.16	4.51		3.44
(2) 0_+	5.01	0.00118	2.90	4.77	0.01033	4.09	4.57	0.00471	2.60
(2) 1	5.21	0.00267	3.02	4.85	0.00174	4.31	4.60	0.00121	3.94
(2) 2	5.65		-3.78	5.52		-4.71	4.84		-3.79
(3) 1	5.70	0.00053	-3.51	5.55	0.00036	-3.70	4.88	0.00462	-3.93
(2) 0_-	5.78		-2.85	5.56		-1.05	5.00		-2.93
(3) 0_+	5.79	0.00073	-2.86	5.66	0.00307	-4.16	5.19	0.01382	-2.45
(3) 0_-	5.88		1.05	5.69		-1.43	5.43		0.32
(4) 1	5.88	0.00019	0.91	5.62	0.00022	0.67	5.06	0.00687	-3.47
(5) 1	6.04	0.01579	-2.89	5.87	0.00871	-1.90	5.45	0.00672	0.18
(6) 1	6.44	0.00007	4.69	5.89	0.00152	4.03	5.77	0.00002	5.15
(3) 2	6.49		4.59	5.91		6.37	5.79		5.10
(4) 0_-	6.65		4.33	6.23		6.24	6.11		5.27
(4) 0_+	6.66	0.04221	2.57	6.31	0.02758	4.31	6.08	0.05780	2.49
(7) 1	6.73	0.00064	3.94	6.38	0.00449	5.98	6.28	0.00264	4.62
(5) 0_-	6.93		0.51	6.46		5.97	6.33		4.59
(1) 3	6.94		4.37	6.36		6.58	6.23		5.37
(8) 1	6.95	0.00003	-1.37	6.85	0.00248	2.78	6.46	2.5E-06	-3.73
(6) 0_-	7.00		1.95	6.92		-2.26	6.62		-3.17
(5) 0_+	7.02	0.01252	4.18	6.53	0.00005	6.13	6.41	0.00099	4.60
(4) 2	7.21		3.89	6.87		5.85	6.59		-3.79
(9) 1	7.25	0.00051	3.75	6.94	0.00172	0.55	6.76	0.00315	4.24
(5) 2	7.39		-3.73	7.22		-4.50	6.73		4.16
(10) 1	7.45	1.1E-06	-3.17	7.30	0.00100	-3.85	6.81	0.00004	-3.26
(11) 1	7.48	0.00024	-3.01	7.31	0.00023	-3.58	6.95	0.00027	-1.60
(6) 0_+	7.50	0.00499	-1.97	7.33	0.21391	-1.94	6.97	0.05845	-1.43
(7) 0_-	7.56		-2.64	7.36		-2.75	6.93		-1.87
(2) 3	7.83		-3.81	7.69		-4.49	7.03		-4.17
(7) 0_+	7.85	0.00259	-3.20	7.61	0.03067	3.07	7.12	0.09376	-2.45
(8) 0_-	7.89		-3.64	7.63		3.06	7.11		-2.96
(6) 2	7.99		-2.92	7.81		-3.82	7.29		-3.11
(9) 0_-	7.99		2.58	7.72		-4.26	7.40		1.29
(8) 0_+	8.00	0.00001	2.61	7.66	0.61485	-2.65	7.38	0.01211	1.03
(12) 1	8.03	0.00601	1.01	7.67	0.01509	2.95	7.34	0.00003	-1.98
(13) 1	8.06	0.00300	-2.01	7.88	0.00425	-3.57	7.43	0.00294	0.33
(9) 0_+	8.16	1.58677	2.45	7.81	1.32056	1.24	7.67	2.53150	1.12
(7) 2	8.46		2.63	8.09		3.68	7.81		1.59
(14) 1	8.48	0.00566	2.02	8.13	0.01668	2.83	7.85	0.00125	1.21

S.III. BENCHMARK ON THE ABSORPTION CROSS SECTION SIMULATIONS

In this section, a possible problem of chosing the proper ensemble of geometries $\boldsymbol{R_k}$ in the absorption cross section simulations is shortly discussed. In this small benchmark, $HgBr_2$ has been chosen as a representative system. Methodological parameters –active space, symmetry restrictions, number of states per IrRep, IPEA and IMAG shifts, and Gaussian broadening δ– are the same as those reported in Section II.

A. Equilibrium structures used in the generation of the Wigner distributions

The first issue is related to the information on the ground–state equilibrium structures –optimized geometries and vibrational frequencies of the normal modes– used in the process of generating the set of geometries by using the Wigner distribution. In this benchmark, the method for determining the vertical excitation energies ΔE and f has been kept unchanged – they are computed at the same level of theory, namely DKH3–SOC–MS–CASPT2(12,10)/ANO–RCC. The methodologies used to determine the gradients and Hessians for the ground–state structures are the following:

- cheap and low–level DFT with the PBE0/Def2QZVP level, which is a good candidate for the optimizations of structures of the larger mercury–based molecules[1]
- DKH3–CASPT2(12,10)/ANO–RCC–V(T/Q)ZP consistent with the further computations of ΔE and f at the same level of theory
- CCSD, which is a typical reference in these type of optimization procedures, along with the Def2QZVP basis set

In the case of DFT/PBE0, CCSD, and CASPT2, the ANO–RCC–VTZP basis set is used and later the results are compared with those provided with the CASPT2 method and the larger ANO–RCC–VQZP basis set.

When comparing just the equilibrium R_{HgBr} bond lengths and vibrational frequencies (see Table S.1), it can be easily observed that the CASPT2(12,10)/ANO–RCC–VQZP methodology is actually performing less accurately than the other protocols. This problem was already highlighted in our first benchmark paper on the spectral properties of IBr and

$HgBr_2$[20] and it is related to the fact that the ground–state wavefunction of $HgBr_2$ has basically one–reference character and thus CASPT2 performs just as regular MP2 method. However, the final outcome of the usage of CASPT2 geometries in the $\sigma(E)$ simulations is almost the same as in the case of DFT/PBE0 or CCSD methods (see Figure S1). Firstly, the values of $\sigma(E)$ are of the same magnitude for all bands. Secondly, the shifts of the bands are negligible and much less than the uncertainty between the experimental measurements of Roxlo[21] and Maya.[22] Among them, the largest shifts (up to 0.25 eV) are noticed for the first band a, which still has very broad and uncertain shape. Small differences are observed for band b, for which the use of the ensemble of DFT/PBE0 geometries leads to the sharpest band shape. Only in the case of CCSD/Def2QZVP and CASPT2(12,10)/ANO–RCC–VQZP ensembles the side small right–side peak at ≈ 6.46 eV is noticed. For the DFT/Def2QZVP and CASPT2(12,10)/ANO–RCC–VTZP the peak is less pronounced and becomes a shoulder of band b. This has not been reported experimentally, due to the larger experimental broadening of this band. Moreover, a perfect agreement is observed for band c, for which in the case of all R_k ensembles, the same position, shape, and intensity are predicted. Lastly, there are not any other differences than those pointed out above if the ANO–RCC–VTZP or ANO–RCC–VQZP basis sets are used in the CASPT2 geometry optimization and ΔE and f computations. This is promising for future computations of these cross sections for larger mercury systems, for which smaller basis set (of a triple–ζ quality) could easily be used.

In conclusion, a good feature of the $\sigma(E)$ simulation technique based on statistical averaging is that, despite noticeable differences in the equilibrium structure properties, the final outcome of the simulation seems to be invariant on the quantum–chemical method used to generate the ensemble of Wigner geometries.

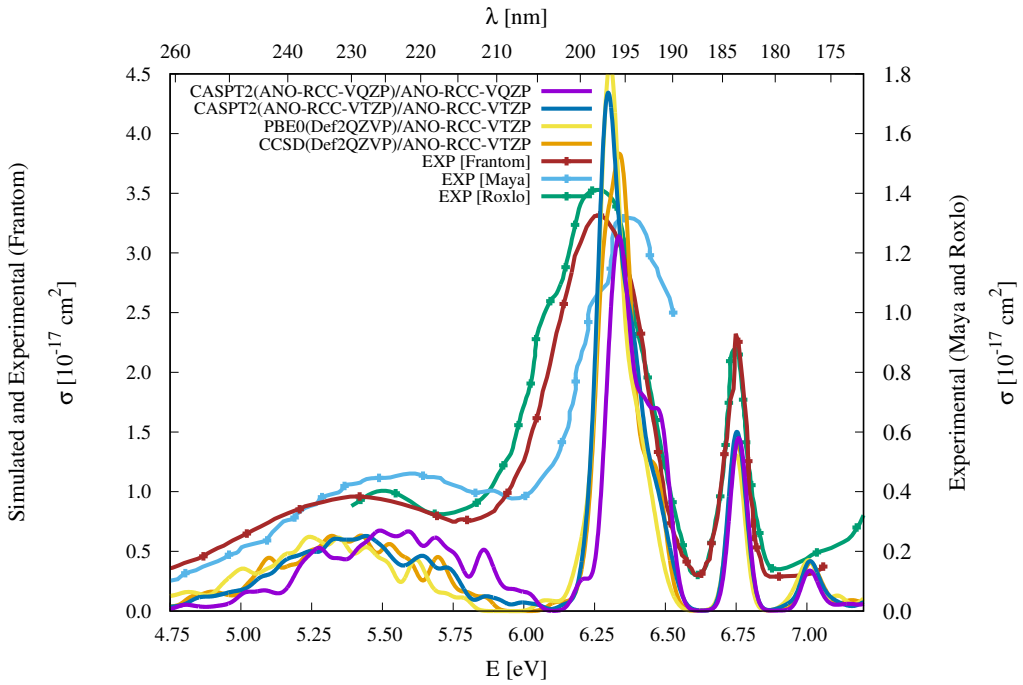

FIG. S.1: Simulated absorption spectra of $HgBr_2$ arising from different sampling of Wigner geometries. In the legend, the method used in the geometry optimization of the ground state and the computation of the vibrational frequencies is on the left, whereas on the right the basis set used in the DKH3–SOC–MS–CASPT2(12,10) computations of ΔE and f is given. Experimental spectra[21–23] are included for the comparison (for better comparison, the $\sigma(E)$ values of spectrum of Frantom *et al.*[23] shown on the same axis as theoretical ones).

B. Number of sampled geometries

In this benchmark, the convergence of the obtained absorption cross sections upon increasing the number of geometries used in the averaging procedure is tested. Both equilibrium structure and the ΔE and f data are obtained at the same level of theory, DKH3–SOC–MS–CASPT2(12,10)/ANO–RCC–VQZP. The results of the simulations using N_p=25, 50, 75, and 100 geometries in the ensemble are presented in Figure S.2. It can be easily noticed that the convergence of $\sigma(E)$ is reached fairly quickly, with basically no observable differences in the spectra, i.e. no shifts of bands are noticed and only minor changes in the bands curvature are observed. Moreover, they affect mostly the broad band a and the right–side peak of main band b (observed at 6.46 eV). Even with very small and insufficient number of sampled geometries N_p=25, the qualitative picture of the spectrum is still conserved (although this would be true only for such small triatomic system). It is worth mentioning that the statistical errors of the sampling $\delta\sigma(E)$ (not shown in Figure S2) decreases with the number

of the sampled geometries, which can be already predicted by the form of Equation 3.

In conclusion, the chosen number of sampled geometries N_p=100 is proved to be completely reliable.

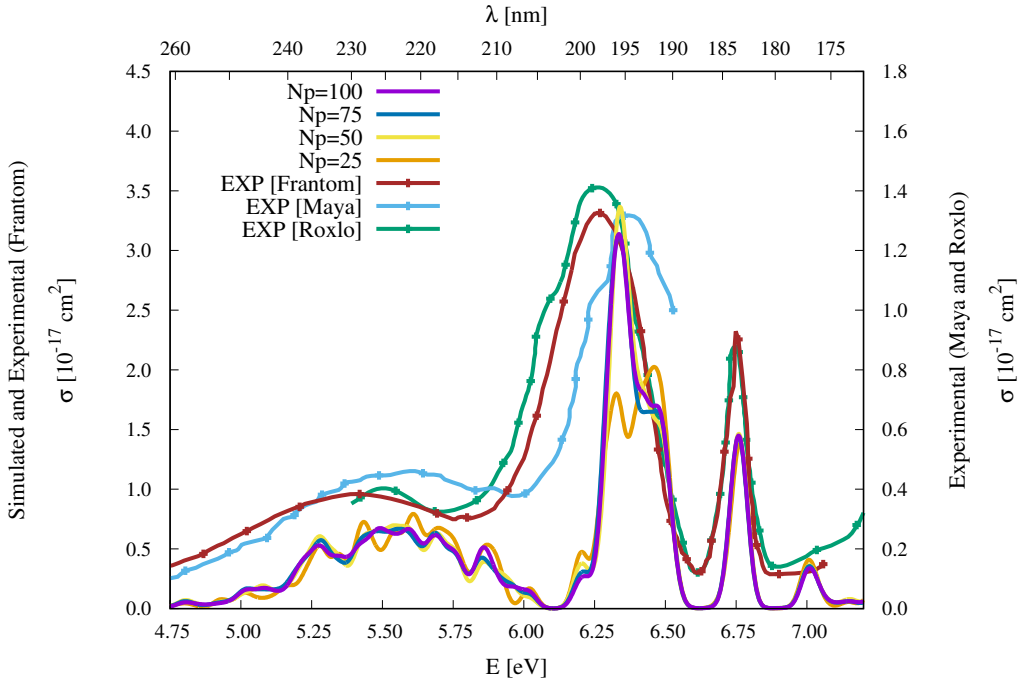

FIG. S.2: Convergence of the DKH3–SOC–MSCASPT2(12,10)/ANO–RCC–VQZP simulated spectra of $HgBr_2$ with different number of sampled geometries (N_p). Sampled geometries were obtained with the Wigner distribution using DKH3–CASPT2(12,10)/ANO–RCC–VQZP equilibrium structure. Experimental spectra[21–23] are included for the comparison (for better comparison, the $\sigma(E)$ values of spectrum of Frantom *et al.*[23] shown on the same axis as theoretical ones).

S.IV. SIMULATED UV–VIS ABSORPTION CROSS SECTIONS OF HGXY

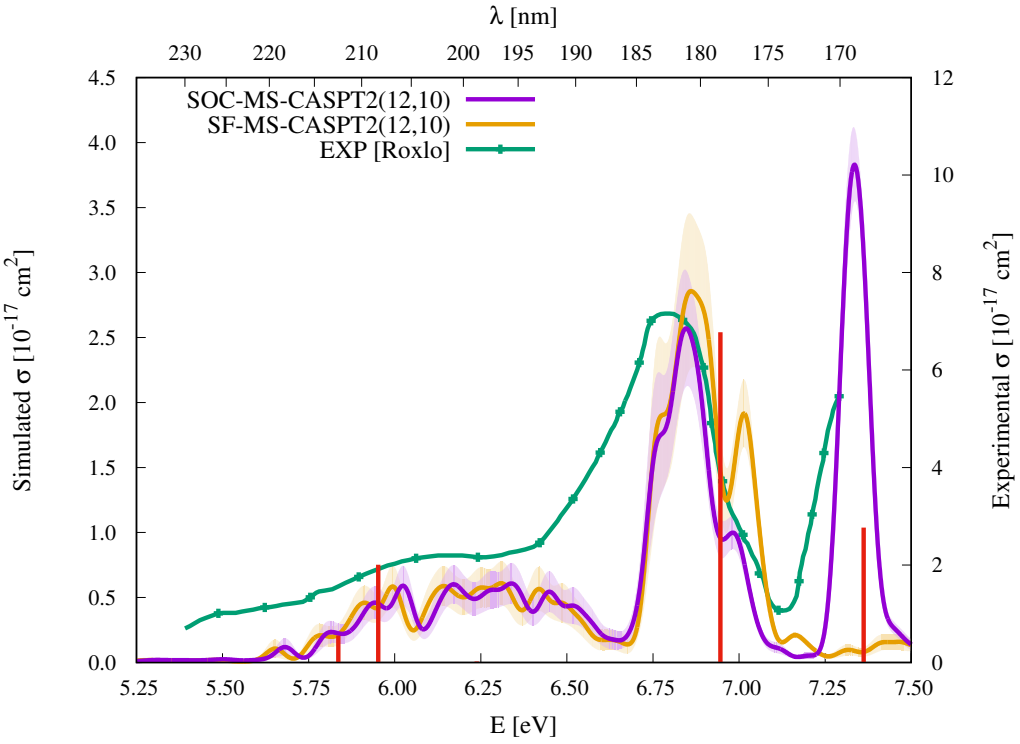

FIG. S.3: Simulated UV–Vis absorption cross sections ($\sigma(E)$) of $HgCl_2$ both without (SF, orange) and with (SOC, violet) taking into account the spin–orbit coupling between states. Shaded areas represent the statistical error for the sampled photon energies ($\delta\sigma(E)$). Experimental spectrum[21] is included for the comparison. Additionally, vertical excitation energies in eV (ΔE) and associated f values between SO states for the optimized ground–state structure of $HgCl_2$ are graphically represented with red sticks (see the discussion in Section II).

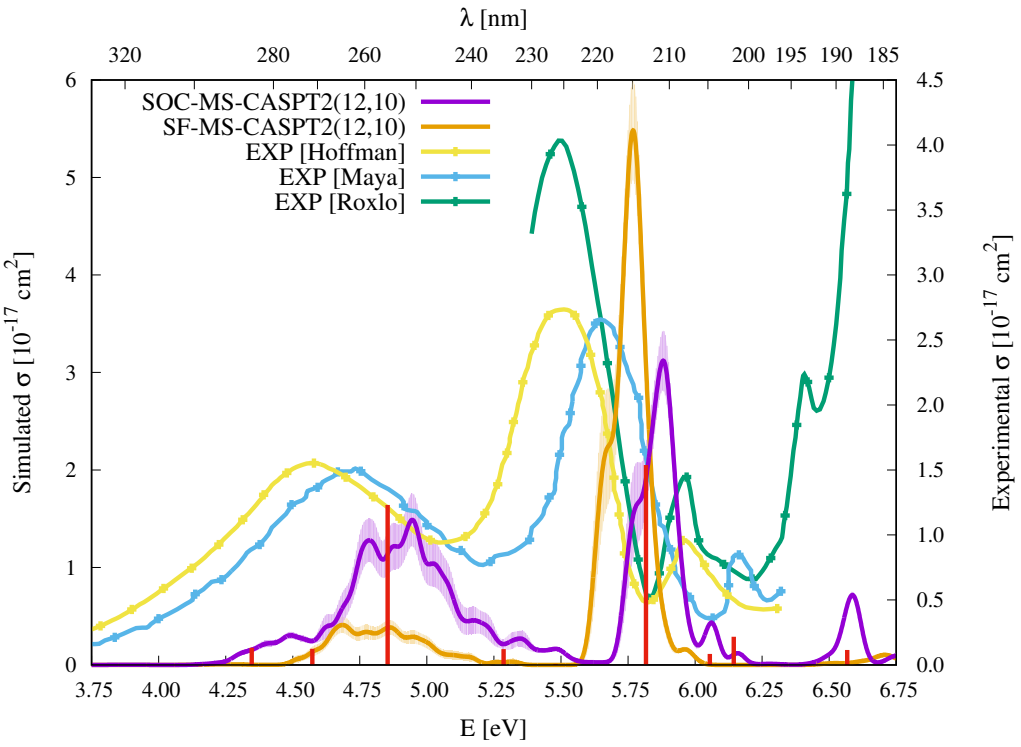

FIG. S.4: Simulated UV–Vis absorption cross sections ($\sigma(E)$) of HgI_2 both without (SF, orange) and with (SOC, violet) taking into account the spin–orbit coupling between states. Shaded areas represent the statistical error for the sampled photon energies ($\delta\sigma(E)$). Experimental spectra[21,22,24] are included for the comparison. Additionally, vertical excitation energies in eV (ΔE) and associated f values between SO states for the optimized ground–state structure of HgI_2 are graphically represented with red sticks (see the discussion in Section II).

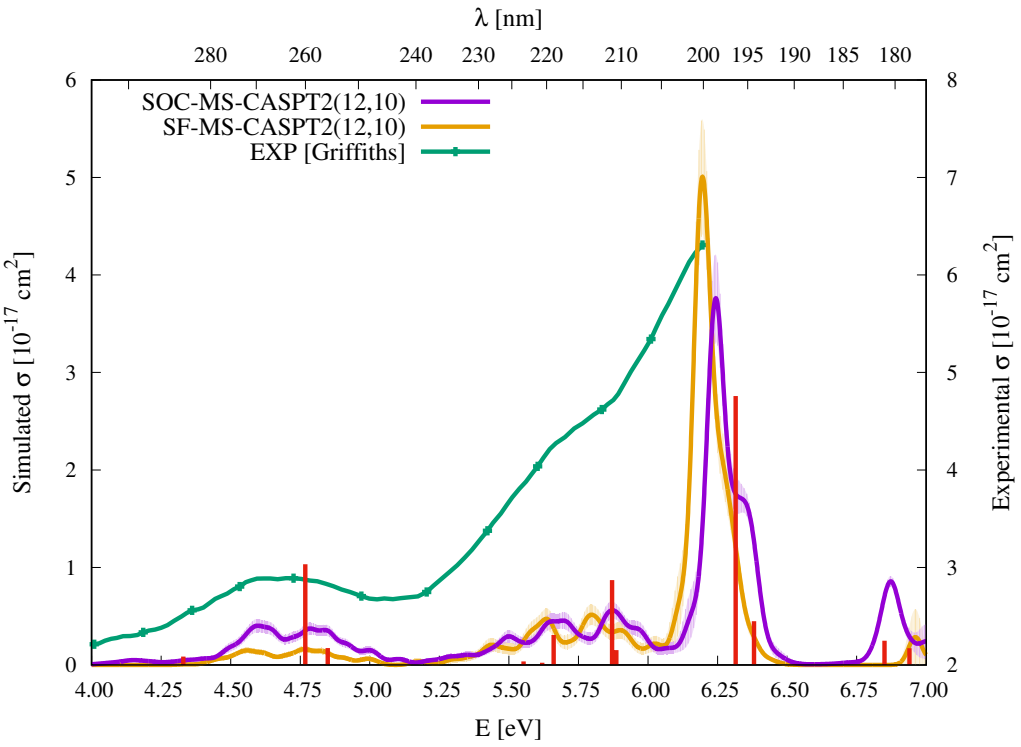

FIG. S.5: Simulated UV–Vis absorption cross sections ($\sigma(E)$) of HgClI both without (SF, orange) and with (SOC, violet) taking into account the spin–orbit coupling between states. Shaded areas represent the statistical error for the sampled photon energies ($\delta\sigma(E)$). Experimental spectrum[25] is included for the comparison. Additionally, vertical excitation energies in eV (ΔE) and associated f values between SO states for the optimized ground–state structure of HgClI are graphically represented with red sticks (see the discussion in Section II).

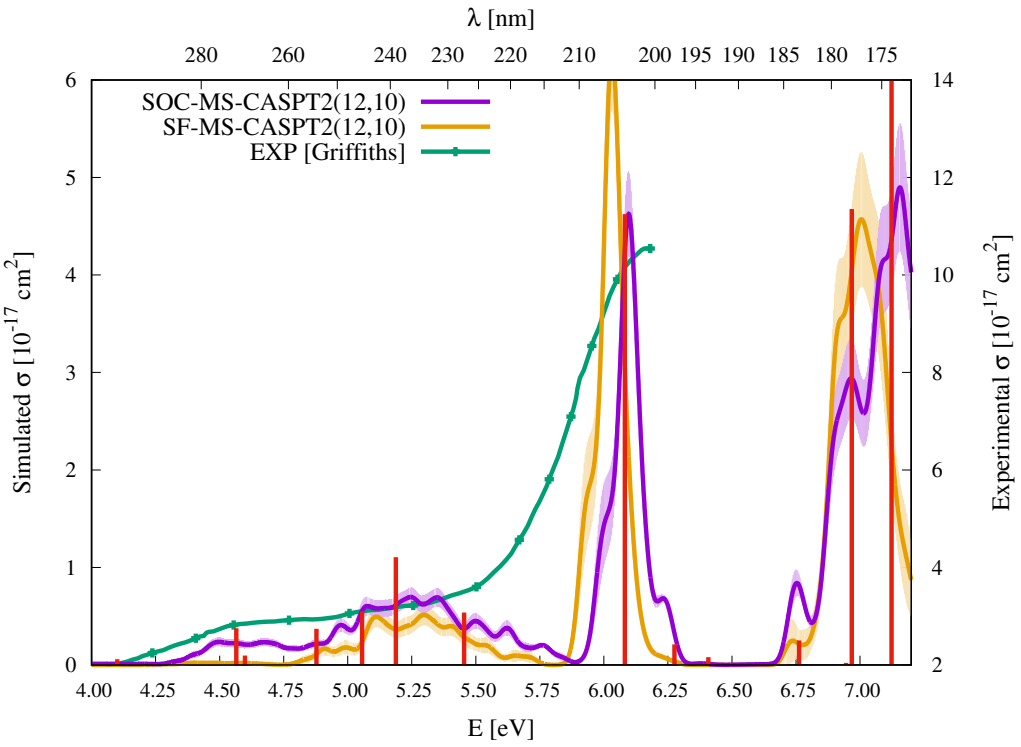

FIG. S.6: Simulated UV–Vis absorption cross sections ($\sigma(E)$) of HgBrI both without (SF, orange) and with (SOC, violet) taking into account the spin–orbit coupling between states. Shaded areas represent the statistical error for the sampled photon energies ($\delta\sigma(E)$). Experimental spectrum[25] is included for the comparison. Additionally, vertical excitation energies in eV (ΔE) and associated f values between SO states for the optimized ground–state structure of HgBrI are graphically represented with red sticks (see the discussion in Section II).

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