Electronic Supplementary Material (ESI) for Photochemical & Photobiological Science

A theoretical study of thionine: Spin-orbit coupling and intersystem crossing

Electronic Supporting Information

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Table S1 Calculated rate constants k_{ISC} for the $S_1 \rightarrow T_{1x}$ channel. Remaining columns: adiabatic energy difference ΔE^{ad}, number of derivatives with respect of out-of-plane modes ($\#_{derivs}$), width of the search interval η, number of accepting modes within the search interval ($\#_{acc}$) and number of final state vibrational levels within the search interval ($\#_{v'}$).

Channel	ΔE^{ad}/eV	vibr. SO $\#_{derivs}$	Acceptors $\#_{acc}$	Interval η/cm^{-1}	Levels $\#_{v'}$	k_{ISC}/s^{-1}
$S_1 \rightarrow T_{1x}$	0.64	12	25	0.001	5×10^2	1.07×10^0
$S_1 \rightarrow T_{1x}$	0.64	12	25	0.01	6×10^3	4.43×10^1
$S_1 \rightarrow T_{1x}$	0.64	12	25	0.1	6×10^4	2.73×10^3
$S_1 \rightarrow T_{1x}$	0.64	12	25	1	6×10^5	1.96×10^3
$S_1 \rightarrow T_{1x}$	0.64	12	25	10	6×10^6	2.57×10^3
$S_1 \rightarrow T_{1x}$	0.64	12	25	100	6×10^7	3.28×10^3
$S_1 \rightarrow T_{1x}$	0.64	12	49	0.001	3×10^4	2.75×10^3
$S_1 \rightarrow T_{1x}$	0.64	12	49	0.01	3×10^5	3.36×10^5
$S_1 \rightarrow T_{1x}$	0.64	12	49	0.1	3×10^6	2.40×10^5
$S_1 \rightarrow T_{1x}$	0.64	12	49	1	3×10^7	3.63×10^5
$S_1 \rightarrow T_{1x}$	0.64	12	49	10	1×10^8	7.51×10^5

Table S2 Calculated rate constants k_{ISC} for the $S_1 \rightarrow T_{1z}$ channel. Remaining columns: adiabatic energy difference ΔE^{ad}, number of derivatives with respect of out-of-plane modes ($\#_{derivs}$), width of the search interval η, number of accepting modes within the search interval ($\#_{acc}$) and number of final state vibrational levels within the search interval ($\#_{v'}$).

Channel	ΔE^{ad}/eV	vibr. SO $\#_{derivs}$	Acceptors $\#_{acc}$	Interval η/cm^{-1}	Levels $\#_{v'}$	k_{ISC}/s^{-1}
$S_1 \rightarrow T_{1z}$	0.64	11	25	0.001	4×10^2	1.66×10^1
$S_1 \rightarrow T_{1z}$	0.64	11	25	0.01	4×10^3	1.27×10^2
$S_1 \rightarrow T_{1z}$	0.64	11	25	0.1	4×10^4	3.62×10^3
$S_1 \rightarrow T_{1z}$	0.64	11	25	1	4×10^5	5.10×10^3
$S_1 \rightarrow T_{1z}$	0.64	11	25	10	4×10^6	3.96×10^3
$S_1 \rightarrow T_{1z}$	0.64	11	25	100	4×10^7	4.31×10^3
$S_1 \rightarrow T_{1z}$	0.64	11	49	0.001	2×10^4	4.51×10^4
$S_1 \rightarrow T_{1z}$	0.64	11	49	0.01	2×10^5	1.98×10^5
$S_1 \rightarrow T_{1z}$	0.64	11	49	0.1	2×10^6	2.14×10^5
$S_1 \rightarrow T_{1z}$	0.64	11	49	1	2×10^7	4.15×10^6
$S_1 \rightarrow T_{1z}$	0.64	11	49	10	1×10^7	1.56×10^5

Table S3 Calculated rate constants k_{ISC} for the $S_1 \rightarrow T_{2x}$ channel. Remaining columns: adiabatic energy difference ΔE^{ad}, number of derivatives with respect of out-of-plane modes ($\#_{derivs}$), width of the search interval η, number of accepting modes within the search interval ($\#_{acc}$) and number of final state vibrational levels within the search interval ($\#_{v'}$).

Channel	ΔE^{ad}/eV	vibr. SO $\#_{derivs}$	Acceptors $\#_{acc}$	Interval η/cm^{-1}	Levels $\#_{v'}$	k_{ISC}/s^{-1}
$S_1 \rightarrow T_{2x}$	0.30	11	25	0.001	6	2.27×10^6
$S_1 \rightarrow T_{2x}$	0.30	11	25	0.01	33	1.50×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	25	0.1	3×10^2	9.73×10^7
$S_1 \rightarrow T_{2x}$	0.30	11	25	1	3×10^3	1.03×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	25	10	3×10^4	1.28×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	25	100	3×10^5	1.40×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	49	0.001	42	4.86×10^7
$S_1 \rightarrow T_{2x}$	0.30	11	49	0.01	5×10^2	1.96×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	49	0.1	5×10^3	1.55×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	49	1	5×10^4	2.81×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	49	10	5×10^5	2.79×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	49	100	5×10^6	2.94×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	72	0.001	9×10^3	5.16×10^7
$S_1 \rightarrow T_{2x}$	0.30	11	72	0.01	9×10^4	2.06×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	72	0.1	9×10^5	1.89×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	72	1	9×10^6	3.13×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	72	10	2×10^7	3.07×10^8
$S_1 \rightarrow T_{2x}$	0.30	11	72	100	2×10^8	3.23×10^8
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	25	0.001	6	4.69×10^5
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	25	0.01	33	3.51×10^7
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	25	0.1	3×10^2	9.52×10^7
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	25	1	3×10^3	3.11×10^7
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	25	10	3×10^4	4.00×10^7
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	25	100	3×10^5	5.10×10^7
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	49	0.001	42	1.46×10^7
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	49	0.01	5×10^2	1.24×10^8
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	49	0.1	5×10^3	1.28×10^8
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	49	1	5×10^4	1.44×10^8
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	49	10	5×10^5	1.04×10^8
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	49	100	5×10^6	1.12×10^8
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	72	0.001	9×10^3	1.59×10^7
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	72	0.01	9×10^4	1.30×10^8
$S_1 \rightarrow T_{2x}$	0.30	1 (v_1)	72	0.1	9×10^5	1.43×10^8
$S_1 \rightarrow T_{2x}$	0.30	6	25	0.001	6	2.30×10^6
$S_1 \rightarrow T_{2x}$	0.30	6	25	0.01	33	1.53×10^8
$S_1 \rightarrow T_{2x}$	0.30	6	25	0.1	3×10^2	1.07×10^8
$S_1 \rightarrow T_{2x}$	0.30	6	25	1	3×10^3	9.81×10^7
$S_1 \rightarrow T_{2x}$	0.30	6	25	10	3×10^4	1.26×10^8
$S_1 \rightarrow T_{2x}$	0.30	6	25	100	3×10^5	1.26×10^8
$S_1 \rightarrow T_{2x}$	0.30	6	49	0.001	42	4.72×10^7
$S_1 \rightarrow T_{2x}$	0.30	6	49	0.01	5×10^2	1.88×10^8
$S_1 \rightarrow T_{2x}$	0.30	6	49	0.1	5×10^3	1.62×10^8
$S_1 \rightarrow T_{2x}$	0.30	6	49	1	5×10^4	2.76×10^8
$S_1 \rightarrow T_{2x}$	0.30	6	49	10	5×10^5	2.72×10^8
$S_1 \rightarrow T_{2x}$	0.30	6	49	100	5×10^6	2.73×10^8

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Table S4 Calculated rate constants k_{ISC} for the $S_1 \rightarrow T_{2z}$ channel. Remaining columns: adiabatic energy difference ΔE^{ad}, number of derivatives with respect of out-of-plane modes ($\#_{derivs}$), width of the search interval η, number of accepting modes within the search interval ($\#_{acc}$) and number of final state vibrational levels within the search interval ($\#_{v'}$).

Channel	ΔE^{ad}/eV	vibr. SO $\#_{derivs}$	Acceptors $\#_{acc}$	Interval η/cm^{-1}	Levels $\#_{v'}$	k_{ISC}/s^{-1}
$S_1 \rightarrow T_{2z}$	0.30	12	25	0.001	3	2.87×10^{2}
$S_1 \rightarrow T_{2z}$	0.30	12	25	0.01	33	2.49×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	12	25	0.1	4×10^{2}	1.93×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	12	25	1	4×10^{3}	7.70×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	12	25	10	4×10^{4}	6.34×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	12	25	100	4×10^{5}	2.93×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	12	49	0.001	28	2.14×10^{3}
$S_1 \rightarrow T_{2z}$	0.30	12	49	0.01	3×10^{2}	2.67×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	12	49	0.1	4×10^{3}	6.30×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	12	49	1	4×10^{4}	9.16×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	12	49	10	4×10^{5}	1.60×10^{8}
$S_1 \rightarrow T_{2z}$	0.30	12	49	100	4×10^{6}	1.98×10^{8}
$S_1 \rightarrow T_{2z}$	0.30	12	72	0.001	5×10^{3}	7.32×10^{6}
$S_1 \rightarrow T_{2z}$	0.30	12	72	0.01	5×10^{4}	8.81×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	12	72	0.1	1×10^{5}	1.39×10^{8}
$S_1 \rightarrow T_{2z}$	0.30	12	72	1	1×10^{6}	1.39×10^{8}
$S_1 \rightarrow T_{2z}$	0.30	12	72	10	5×10^{7}	2.33×10^{8}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	25	0.001	3	1.39×10^{3}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	25	0.01	33	2.69×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	25	0.1	4×10^{2}	3.65×10^{6}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	25	1	4×10^{3}	1.15×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	25	10	4×10^{4}	2.97×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	25	100	4×10^{5}	3.70×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	49	0.001	28	1.54×10^{3}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	49	0.01	3×10^{2}	2.74×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	49	0.1	4×10^{3}	1.48×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	49	1	4×10^{4}	3.60×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	49	10	4×10^{5}	8.66×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_8)	49	100	4×10^{6}	1.20×10^{8}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	25	0.001	3	6.63×10^{1}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	25	0.01	33	1.42×10^{3}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	25	0.1	4×10^{2}	3.13×10^{5}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	25	1	4×10^{3}	6.33×10^{6}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	25	10	4×10^{4}	1.05×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	25	100	4×10^{5}	1.25×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	49	0.001	28	1.62×10^{2}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	49	0.01	3×10^{2}	9.59×10^{4}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	49	0.1	4×10^{3}	1.67×10^{6}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	49	1	4×10^{4}	3.71×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	49	10	4×10^{5}	4.00×10^{7}
$S_1 \rightarrow T_{2z}$	0.30	1 (v_{20})	49	100	4×10^{6}	2.99×10^{7}

Table S5 Harmonic frequencies v_i of the A" *out-of-plane* vibrational modes for the S_2 ($\pi_{H-1}\rightarrow\pi_L$*) state. Derivatives of the SOMEs with respect to the corresponding (dimensionless) normal coordinates at the S_2 ($\pi_{H-1}\rightarrow\pi_L$*) DFT/MRCI minimum.

Modes	$\bar{v}_i\,/\,cm^{-1}$	$\frac{\partial\langle S_2\vert\hat{H}_{SO}\vert T_{1x}\rangle}{\partial q_i}$	$\frac{\partial\langle S_2\vert\hat{H}_{SO}\vert T_{1y}\rangle}{\partial q_i}$	$\frac{\partial\langle S_2\vert\hat{H}_{SO}\vert T_{2x}\rangle}{\partial q_i}$	$\frac{\partial\langle S_2\vert\hat{H}_{SO}\vert T_{2y}\rangle}{\partial q_i}$
1	20.0	-0.18	1.31	1.97	-0.62
2	43.5	0.03	-0.21	-0.19	0.12
3	78.8	0.52	-0.02	-0.44	0.06
4	153.1	0.20	-0.18	-0.37	0.11
6	170.1	-0.08	0.31	0.05	0.05
7	181.9	-0.05	-0.03	-0.02	-0.08
9	250.5	-0.16	-0.05	0.10	0.04
10	269.5	0.31	0.09	-0.37	-0.15
11	291.5	0.09	1.10	-0.17	-0.82
13	317.6	0.39	0.27	-0.44	-0.33
15	386.5	0.41	0.64	-0.37	-0.36
17	398.5	0.48	-0.28	-0.60	0.20
18	429.1	-0.61	-0.60	0.63	0.67
20	433.8	-0.32	0.65	0.17	-0.56
23	534.6	-0.06	0.11	-0.18	-0.33
24	545.6	-0.20	0.01	0.08	-0.01
25	555.1	0.18	0.34	0.00	-0.40
29	747.7	-0.37	-0.72	0.48	0.32
30	788.9	0.43	-0.46	-0.28	0.26
32	831.5	0.41	0.06	-0.45	-0.10
33	836.3	0.12	0.47	-0.26	-0.39
37	924.4	-0.29	-0.10	0.39	0.10
38	928.1	-0.01	0.16	-0.22	-0.04

Table S6 Calculated rate constants k_{ISC} for the $S_2\rightarrow T_{i(x/y)}$ (i = 1, 2) channels. Remaining columns: adiabatic energy difference ΔE^{ad}, number of derivatives with respect of out-of-plane modes ($\#_{derivs}$), width of the search interval η, number of accepting modes within the search interval ($\#_{acc}$) and number of final state vibrational levels within the search interval ($\#_{v'}$).

Channel	ΔE^{ad}/eV	vibr. SO $\#_{derivs}$	Acceptors $\#_{acc}$	Interval η/cm^{-1}	Levels $\#_{v'}$	k_{ISC}/s^{-1}
$S_2\rightarrow T_{1x}$	0.66	23	49	0.001	2×10^2	2.10×10^4
$S_2\rightarrow T_{1x}$	0.66	23	49	0.01	2×10^3	6.53×10^5
$S_2\rightarrow T_{1x}$	0.66	23	49	0.1	2×10^4	5.71×10^6
$S_2\rightarrow T_{1x}$	0.66	23	49	1	2×10^5	5.56×10^6
$S_2\rightarrow T_{1x}$	0.66	23	49	10	2×10^6	3.17×10^6
$S_2\rightarrow T_{1x}$	0.66	23	49	100	-	-
$S_2\rightarrow T_{1y}$	0.66	23	49	0.001	2×10^2	4.53×10^4
$S_2\rightarrow T_{1y}$	0.66	23	49	0.01	2×10^3	1.64×10^6
$S_2\rightarrow T_{1y}$	0.66	23	49	0.1	2×10^4	4.02×10^6
$S_2\rightarrow T_{1y}$	0.66	23	49	1	2×10^5	8.63×10^6
$S_2\rightarrow T_{1y}$	0.66	23	49	10	2×10^6	5.67×10^6
$S_2\rightarrow T_{1y}$	0.66	23	49	100	-	-
$S_2\rightarrow T_{2x}$	0.66	23	49	0.001	0	-
$S_2\rightarrow T_{2x}$	0.32	23	49	0.01	3	3.91×10^1
$S_2\rightarrow T_{2x}$	0.32	23	49	0.1	41	5.14×10^5
$S_2\rightarrow T_{2x}$	0.32	23	49	1	4×10^2	7.40×10^6
$S_2\rightarrow T_{2x}$	0.32	23	49	10	5×10^3	3.22×10^6
$S_2\rightarrow T_{2x}$	0.32	23	49	100	5×10^4	2.62×10^6
$S_2\rightarrow T_{2y}$	0.32	23	49	0.001	0	-
$S_2\rightarrow T_{2y}$	0.32	23	49	0.01	3	1.63×10^3
$S_2\rightarrow T_{2y}$	0.32	23	49	0.1	41	9.43×10^4
$S_2\rightarrow T_{2y}$	0.32	23	49	1	4×10^2	2.68×10^5
$S_2\rightarrow T_{2y}$	0.32	23	49	10	5×10^3	4.03×10^6
$S_2\rightarrow T_{2y}$	0.32	23	49	100	5×10^4	3.58×10^6

Table S7 Calculated rate constants k_{ISC} for the $S_1 \rightarrow T_{i(x/z)}$ (i = 1, 2) channel varying the adiabatic energy difference ΔE^{ad}. Remaining columns: number of derivatives with respect of out-of-plane modes ($\#_{derivs}$), width of the search interval η, number of accepting modes within the search interval ($\#_{acc}$) and number of final state vibrational levels within the search interval ($\#_{v'}$).

Channel	ΔE^{ad}/eV	vibr. SO $\#_{derivs}$	Acceptors $\#_{acc}$	Interval η/cm^{-1}	Levels $\#_{v'}$	k_{ISC}/s^{-1}
$S_1 \rightarrow T_{1x}$	0.68	12	49	0.001	7 x 10^4	1.34 x 10^4
$S_1 \rightarrow T_{1x}$	0.68	12	49	0.01	7 x 10^5	2.05 x 10^4
$S_1 \rightarrow T_{1x}$	0.68	12	49	0.1	7 x 10^6	3.06 x 10^5
$S_1 \rightarrow T_{1x}$	0.68	12	49	1	7 x 10^7	2.44 x 10^5
$S_1 \rightarrow T_{1z}$	0.68	11	49	0.001	5 x 10^4	2.04 x 10^4
$S_1 \rightarrow T_{1z}$	0.68	11	49	0.01	5 x 10^5	2.54 x 10^5
$S_1 \rightarrow T_{1z}$	0.68	11	49	0.1	5 x 10^6	1.27 x 10^6
$S_1 \rightarrow T_{1z}$	0.68	11	49	1	5 x 10^7	4.00 x 10^5
$S_1 \rightarrow T_{2x}$	0.19	11	49	0.001	4	3.60 x 10^5
$S_1 \rightarrow T_{2x}$	0.19	11	49	0.01	41	2.08 x 10^8
$S_1 \rightarrow T_{2x}$	0.19	11	49	0.1	5 x 10^2	7.79 x 10^7
$S_1 \rightarrow T_{2x}$	0.19	11	49	1	5 x 10^3	1.31 x 10^9
$S_1 \rightarrow T_{2x}$	0.21	11	49	0.001	3	8.41 x 10^4
$S_1 \rightarrow T_{2x}$	0.21	11	49	0.01	78	3.49 x 10^7
$S_1 \rightarrow T_{2x}$	0.21	11	49	0.1	8 x 10^2	1.29 x 10^9
$S_1 \rightarrow T_{2x}$	0.21	11	49	1	8 x 10^3	6.21 x 10^8
$S_1 \rightarrow T_{2x}$	0.22	11	49	0.01	1 x 10^2	6.22 x 10^8
$S_1 \rightarrow T_{2x}$	0.22	11	49	0.1	1 x 10^3	2.12 x 10^8
$S_1 \rightarrow T_{2x}$	0.22	11	49	1	1 x 10^4	1.98 x 10^8
$S_1 \rightarrow T_{2x}$	0.31	11	49	0.001	90	9.33 x 10^6
$S_1 \rightarrow T_{2x}$	0.31	11	49	0.01	9 x 10^2	1.94 x 10^7
$S_1 \rightarrow T_{2x}$	0.31	11	49	0.1	9 x 10^3	7.72 x 10^7
$S_1 \rightarrow T_{2x}$	0.31	11	49	1	9 x 10^4	3.04 x 10^8
$S_1 \rightarrow T_{2z}$	0.19	12	49	0.001	6	2.69 x 10^3
$S_1 \rightarrow T_{2z}$	0.19	12	49	0.01	41	3.36 x 10^6
$S_1 \rightarrow T_{2z}$	0.19	12	49	0.1	4 x 10^2	1.08 x 10^7
$S_1 \rightarrow T_{2z}$	0.19	12	49	1	4 x 10^3	4.69 x 10^7
$S_1 \rightarrow T_{2z}$	0.21	12	49	0.001	5	9.88 x 10^3
$S_1 \rightarrow T_{2z}$	0.21	12	49	0.01	75	2.46 x 10^5
$S_1 \rightarrow T_{2z}$	0.21	12	49	0.1	6 x 10^2	3.72 x 10^6
$S_1 \rightarrow T_{2z}$	0.21	12	49	1	6 x 10^3	9.39 x 10^7
$S_1 \rightarrow T_{2z}$	0.22	12	49	0.001	13	4.34 x 10^1
$S_1 \rightarrow T_{2z}$	0.22	12	49	0.01	91	5.47 x 10^6
$S_1 \rightarrow T_{2z}$	0.22	12	49	0.1	9 x 10^2	1.42 x 10^7
$S_1 \rightarrow T_{2z}$	0.22	12	49	1	9 x 10^3	5.24 x 10^8
$S_1 \rightarrow T_{2z}$	0.31	12	49	0.001	80	2.00 x 10^5
$S_1 \rightarrow T_{2z}$	0.31	12	49	0.01	7 x 10^2	4.49 x 10^7
$S_1 \rightarrow T_{2z}$	0.31	12	49	0.1	7 x 10^3	1.50 x 10^8
$S_1 \rightarrow T_{2z}$	0.31	12	49	1	7 x 10^4	6.96 x 10^7