

Supporting Information

I.

This section lists Cartesian coordinates (Angstroms) corresponding to optimized molecular geometries of **1-4** in the ground electronic state, S_1 , T_1 and T_2 .

Geometry of **1** optimized in the ground electronic state using B3LYP/aug-cc-pVTZ.

C	-1.448923	0.739898	-0.134206
C	-0.106774	0.592566	-0.095825
C	0.522317	1.920553	-0.133085
C	-0.932542	4.204456	-0.132853
C	-2.402024	4.195756	-0.095640
C	-2.835909	2.917194	-0.134192
H	0.448047	-0.326349	-0.049048
H	-3.000316	5.086997	-0.049087
H	-3.833474	2.511222	-0.120617
H	-2.238500	0.007436	-0.120572
O	-0.137711	5.107925	-0.106983
O	1.677051	2.259087	-0.107385
N	-1.758540	2.073038	-0.216207
N	-0.602880	2.809225	-0.217664

Geometry of **2** optimized in the ground electronic state using B3LYP/aug-cc-pVTZ.

C	-1.536853	0.654559	-0.049023
C	-0.069363	0.618465	-0.083793
C	0.402843	1.885461	-0.082900
C	-0.926064	4.164475	-0.088828
C	-2.393958	4.200334	-0.082011
C	-2.865631	2.933670	-0.045227
H	0.502746	-0.290731	-0.107490
H	-2.966738	5.109117	-0.105346
H	-3.872322	2.552152	-0.034191
O	-0.080806	5.027751	-0.125215
N	-0.649353	2.767030	-0.038220
N	-1.812365	2.052753	-0.015248
O	-2.382579	-0.209019	-0.045700
H	1.409343	2.266864	-0.107314

Geometry of **3** optimized in the ground electronic state using B3LYP/aug-cc-pVTZ.

C	-1.486101	0.705212	-0.159443
C	-0.142018	0.586686	-0.008528
C	0.459664	1.923344	-0.089359
C	-0.963530	4.149298	-0.098001
C	-2.429593	4.164534	-0.022692
C	-2.885547	2.894084	-0.168875
O	-0.166929	5.051234	0.005776
O	1.612282	2.268521	0.016405
N	-1.805593	2.041800	-0.394175
N	-0.642991	2.785234	-0.351011
C	-3.181687	5.437812	0.160067
H	-2.902238	5.918918	1.099010
H	-2.941446	6.145457	-0.635605
H	-4.259004	5.282120	0.165691
C	-4.285708	2.386631	-0.177705
H	-4.500454	1.827416	-1.088904
H	-4.484634	1.730288	0.670650
H	-4.979438	3.220787	-0.120978
C	-2.533953	-0.353060	-0.163208
H	-3.213306	-0.254180	0.684734
H	-3.131690	-0.318567	-1.074596
H	-2.067368	-1.332296	-0.101432
C	0.696573	-0.629811	0.183890
H	1.251464	-0.570892	1.121846
H	0.101463	-1.541141	0.197978
H	1.438785	-0.717028	-0.611819

Geometry of **4** optimized in the ground electronic state using B3LYP/aug-cc-pVTZ.

C	-1.538833	0.670938	-0.214553
C	-0.085826	0.621187	-0.024321
C	0.399438	1.889629	-0.079584
C	-0.955216	4.109865	-0.029750
C	-2.420677	4.150876	-0.011893
C	-2.889404	2.894436	-0.233603
O	-0.130367	4.979698	0.166346
N	-1.812317	2.041460	-0.458504

N	-0.647560	2.764224	-0.357075
C	-3.167394	5.419682	0.221550
H	-2.866728	5.877044	1.165497
H	-2.953141	6.148538	-0.562640
H	-4.243071	5.256249	0.248085
C	-4.272157	2.355763	-0.295299
H	-4.499094	1.993322	-1.299424
H	-4.382158	1.503161	0.375252
H	-4.992884	3.123399	-0.027060
C	0.634194	-0.666666	0.187352
H	1.696684	-0.511051	0.364567
H	0.219609	-1.205051	1.041064
H	0.525994	-1.321637	-0.679493
C	1.776633	2.425356	0.069936
H	2.117142	2.875284	-0.864257
H	1.801741	3.214256	0.822060
H	2.465974	1.633899	0.351091
O	-2.376521	-0.208397	-0.193667

Geometry of **1** optimized in the S₁ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ.

C	-1.475160	0.705506	-0.137859
C	-0.086805	0.607743	-0.126446
C	0.500708	1.913010	-0.118252
C	-0.940668	4.177557	-0.114851
C	-2.371990	4.229620	-0.123072
C	-2.839369	2.881570	-0.128956
H	0.485230	-0.300669	-0.124803
H	-2.967931	5.121620	-0.129000
H	-3.825858	2.459429	-0.128470
H	-2.281516	0.002085	-0.117323
O	-0.091160	5.069243	-0.105959
O	1.639767	2.317263	-0.110161
N	-1.757833	2.102596	-0.127627
N	-0.637594	2.812432	-0.120584

Geometry of **2** optimized in the S₁ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ.

C	-1.505785	0.639682	-0.052448
C	-0.066345	0.599622	-0.073633
C	0.428862	1.891577	-0.091078
C	-0.957269	4.179388	-0.091733
C	-2.396687	4.219345	-0.072180
C	-2.891859	2.927426	-0.052593
H	0.506168	-0.319795	-0.074730
H	-2.969247	5.138729	-0.073010
H	-3.891101	2.513056	-0.034883
O	-0.049315	4.992012	-0.112646
N	-0.665480	2.746563	-0.080760
N	-1.797438	2.072384	-0.058504
O	-2.413696	-0.173065	-0.033025
H	1.428092	2.305955	-0.109284

Geometry of **3** optimized in the S₁ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ.

C	-1.499270	0.712111	-0.099494
C	-0.099365	0.597645	0.074506
C	0.444980	1.911200	0.244999
C	-0.981600	4.142681	0.236462
C	-2.401647	4.199050	0.060083
C	-2.884658	2.879610	-0.109424
C	-3.203260	5.462291	0.062519
C	-4.279441	2.384357	-0.330680
C	-2.533136	-0.346983	-0.321082
C	0.710797	-0.660079	0.085804
H	-2.537133	6.304367	0.228653
H	-3.717998	5.619362	-0.888194
H	-3.956966	5.464457	0.853236
H	-4.384286	1.859846	-1.279327
H	-4.615089	1.727058	0.470211
H	-4.942991	3.243686	-0.352902
H	-3.284248	-0.361105	0.467259
H	-3.036560	-0.235957	-1.280526
H	-2.033913	-1.311353	-0.319457
H	1.753632	-0.408317	0.257648

H	0.391524	-1.342664	0.876650
H	0.643291	-1.196165	-0.863698
O	-0.147252	5.022702	0.417204
O	1.593471	2.300170	0.426556
N	-1.776890	2.061421	-0.036452
N	-0.664992	2.773008	0.159163

Geometry of **4** optimized in the S₁ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ.

C	-1.550427	0.624445	-0.110041
C	-0.118181	0.601500	-0.023133
C	0.392177	1.930418	0.068199
C	-0.956905	4.147415	0.085489
C	-2.389250	4.170472	-0.001460
C	-2.899591	2.841463	-0.092787
O	-0.102335	5.037034	0.177772
N	-1.849794	2.009522	-0.065987
N	-0.657621	2.762543	0.041380
C	-3.174485	5.425404	0.005581
H	-2.954064	6.008497	0.911650
H	-2.882399	6.064524	-0.840889
H	-4.251848	5.237365	-0.045979
C	-4.297798	2.353774	-0.200464
H	-4.780888	2.761007	-1.100287
H	-4.309719	1.261284	-0.248834
H	-4.890022	2.684174	0.664981
C	0.667140	-0.653438	-0.030139
H	1.744560	-0.465236	0.019670
H	0.376498	-1.291782	0.817419
H	0.445419	-1.237379	-0.935322
C	1.790372	2.418118	0.176073
H	2.382701	2.087988	-0.689409
H	1.802258	3.510602	0.224666
H	2.273447	2.010729	1.075832
O	-2.405185	-0.264977	-0.202303

Geometry of **1** optimized in the T₁ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ.

C	-1.492588	0.739738	-0.131781
C	-0.075289	0.616587	-0.121214
C	0.495013	1.935763	-0.117482
C	-0.929650	4.174007	-0.117315
C	-2.367016	4.213861	-0.121227
C	-2.853973	2.878030	-0.132380
H	0.498452	-0.291050	-0.115390
H	-2.947917	5.116743	-0.115319
H	-3.850394	2.484211	-0.131271
H	-2.271049	0.003892	-0.131760
O	-0.111049	5.065768	-0.106636
O	1.650267	2.301035	-0.107005
N	-1.772358	2.064153	-0.133406
N	-0.622622	2.796266	-0.131177

Geometry of **2** optimized in the T₁ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ.

C	-1.512430	0.692478	-0.052759
C	-0.083924	0.615708	-0.073216
C	0.424641	1.919899	-0.090549
C	-0.950535	4.126526	-0.091093
C	-2.379150	4.203194	-0.071948
C	-2.887573	2.899243	-0.051713
H	0.475102	-0.301112	-0.073740
H	-2.938239	5.119977	-0.072658
H	-3.883704	2.507549	-0.035916
H	1.420686	2.311605	-0.110300
O	-0.065260	4.982406	-0.112457
O	-2.397713	-0.163574	-0.033427
N	-0.661810	2.755724	-0.081535
N	-1.801190	2.063260	-0.059196

Geometry of **3** optimized in the T₁ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ.

C	-1.510194	0.714519	-0.101111
C	-0.094593	0.601472	0.075672
C	0.446883	1.922141	0.247481

C	-0.970859	4.139834	0.238936
C	-2.396149	4.201820	0.061170
C	-2.887032	2.868647	-0.110816
C	-3.190589	5.467253	0.063753
C	-4.292445	2.402094	-0.330754
C	-2.522354	-0.366166	-0.322200
C	0.720539	-0.650677	0.087507
H	-2.528856	6.313014	0.228681
H	-3.705761	5.613232	-0.887423
H	-3.944324	5.460009	0.853120
H	-4.412856	1.879481	-1.279766
H	-4.643303	1.747769	0.467444
H	-4.947207	3.269481	-0.351716
H	-3.277193	-0.395976	0.463579
H	-3.030585	-0.269505	-1.281809
H	-2.012079	-1.325918	-0.319607
H	1.764917	-0.404418	0.257906
H	0.392849	-1.329081	0.877212
H	0.642602	-1.182804	-0.862356
O	-0.163508	5.026595	0.417130
O	1.590095	2.283723	0.427045
N	-1.805920	2.042876	-0.040582
N	-0.665075	2.772984	0.161221

Geometry of **4** optimized in the T₁ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ.

C	-1.566969	0.694114	0.215261
C	-0.104628	0.632250	0.069492
C	0.386331	1.897541	0.176333
C	-0.954459	4.078761	0.083230
C	-2.394617	4.198184	0.077274
C	-2.981209	2.834070	0.401893
C	-3.160342	5.462562	-0.079974
C	-4.230149	2.329084	-0.256507
C	0.608733	-0.667665	-0.149589
C	1.788013	2.421271	0.120197
H	-2.489394	6.289652	-0.295471
H	-3.888367	5.380037	-0.888581

H	-3.714310	5.684726	0.835811
H	-4.090802	2.216542	-1.337562
H	-4.516267	1.363549	0.147557
H	-5.041061	3.035899	-0.088601
H	1.682481	-0.525405	-0.244301
H	0.423128	-1.348829	0.680717
H	0.245176	-1.153319	-1.054691
H	1.901405	3.143306	-0.685777
H	2.044371	2.921833	1.052636
H	2.484730	1.604296	-0.040253
O	-0.126317	4.942240	-0.126226
O	-2.387787	-0.194134	0.173206
N	-1.845319	2.028824	0.427878
N	-0.668311	2.766079	0.467723

Geometry of **1** optimized in the T₂ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ.

C	-1.522081	0.777280	-0.146177
C	-0.117298	0.698234	0.073424
C	0.446405	1.996329	-0.219326
C	-0.896053	4.103598	-0.218813
C	-2.310622	4.141444	0.074067
C	-2.833194	2.835199	-0.147323
H	0.447305	-0.146193	0.422229
H	-2.837539	5.010351	0.421711
H	-3.852288	2.498754	-0.174107
H	-2.257499	-0.004348	-0.173754
O	-0.071878	4.978033	-0.100893
O	1.587251	2.373552	-0.101568
N	-1.814485	2.037316	-0.709029
N	-0.618202	2.799456	-0.713807

Geometry of **2** optimized in the T₂ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ.

C	-1.547410	0.671437	-0.051513
C	-0.098657	0.604972	-0.077640
C	0.426576	1.946280	-0.092079
C	-0.915586	4.147549	-0.091561

C	-2.364501	4.213917	-0.077138
C	-2.889611	2.872697	-0.052776
H	0.466610	-0.307617	-0.104011
H	-2.930530	5.126038	-0.103336
H	-3.892503	2.499272	-0.017380
H	1.429972	2.320032	-0.092328
O	-0.072801	5.006606	-0.126733
O	-2.390630	-0.187897	-0.047948
N	-0.651049	2.780267	-0.049727
N	-1.810980	2.039330	-0.026337

Geometry of **3** optimized in the T₂ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ.

C	-1.579103	0.725001	-0.158147
C	-0.156096	0.662028	0.040132
C	0.388186	1.979091	-0.243164
C	-0.946793	4.079954	-0.291385
C	-2.356435	4.137408	0.015235
C	-2.894155	2.822074	-0.151523
C	-3.077321	5.370875	0.453126
C	-4.336333	2.436949	-0.249108
C	-2.487341	-0.438692	-0.404401
C	0.652123	-0.506065	0.499924
H	-2.370174	6.187328	0.571218
H	-3.828648	5.670654	-0.279883
H	-3.585741	5.211393	1.405112
H	-4.585048	2.121248	-1.264385
H	-4.595595	1.625826	0.430283
H	-4.962621	3.288385	0.006776
H	-3.480506	-0.284623	0.010677
H	-2.596554	-0.619548	-1.476789
H	-2.072635	-1.334016	0.053485
H	1.686617	-0.204131	0.639809
H	0.273332	-0.898089	1.445192
H	0.625883	-1.316945	-0.230652
O	-0.122433	4.957976	-0.218491
O	1.522206	2.366938	-0.116332
N	-1.879917	2.001760	-0.717224

N	-0.677900	2.759621	-0.729768
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Geometry of **4** optimized in the T₂ electronic state using CASSCF[14e,11o]/aug-cc-pVDZ

C	-1.495689	0.712291	0.429379
C	-0.082661	0.606167	0.121934
C	0.399839	1.915822	-0.255047
C	-1.011581	4.079580	-0.412401
C	-2.417361	4.175267	-0.082695
C	-2.886686	2.886798	0.295884
C	-3.202212	5.447255	-0.142769
C	-4.255670	2.405298	0.651496
C	0.715708	-0.649470	0.229879
C	1.723005	2.329086	-0.809830
H	-2.531732	6.279893	-0.337804
H	-3.948559	5.416098	-0.938629
H	-3.723310	5.636319	0.796378
H	-4.601883	1.653724	-0.057273
H	-4.274839	1.954792	1.642739
H	-4.949696	3.242312	0.635020
H	1.540729	-0.530949	0.934384
H	0.080605	-1.461616	0.572935
H	1.143261	-0.925767	-0.735861
H	1.744249	2.257677	-1.900139
H	1.951650	3.356239	-0.539940
H	2.501891	1.679916	-0.414876
O	-0.217218	4.925664	-0.763862
O	-2.283124	-0.126461	0.820225
N	-1.812722	2.037108	0.178130
N	-0.701933	2.732421	-0.235583

Our characterization of an excited electronic state as (π, π^*) is premised upon the fact that the configuration state function with the largest coefficient (absolute value) within the state-averaged CASSCF wave function has an electronic configuration that involves the promotion of an electron from a π to π^* orbital (relative to the ground state) even though other CSFs with different electronic configurations also contribute to the overall wave function, albeit to a smaller extent. A more compact representation of the multi-configurational wave function for each electronic state is possible within the basis of natural orbitals that are specific to the state. Here we list coefficients of top contributing CSFs to the wave function of each electronic state in the natural orbital basis.

Table S1 – Coefficients of dominant CSFs for each excited electronic state of **1-4** in the natural orbital basis. (π, π^*) means that the CSF has an electronic configuration involving excitation of an electron from a π to π^* orbital relative to the ground state. (π, π^*, π, π^*) means that the CSF is doubly excited relative to the ground state.

	1	2	3	4
S1	0.91295 (π, π^*)	0.89735 (π, π^*) -0.14022 (π, π^*, π, π^*) -0.10232 (π, π^*)	-0.89593 (π, π^*) -0.13627 (π, π^*)	-0.77660 (π, π^*) 0.24057 (π, π^*, π, π^*)
S2	-0.85382 (n, π^*) -0.27282 (n, π^*) -0.23285 (n, π^*, π, π^*)	0.83119 (n, π^*) -0.27778 (n, π^*) -0.25302 (n, π^*, π, π^*)	0.84817 (n, π^*) 0.30499 (n, π^*) -0.20463 (n, π^*, π, π^*)	0.85531 (π, π^*) -0.23764 (π, π^*)
S3	0.81722 (n, π^*) 0.32625 (n, π^*) 0.26707 (n, π^*, π, π^*)	-0.64447 (π, π^*, π, π^*) 0.56510 (π, π^*, π, π^*) -0.28937 (π, π^*, π, π^*)	0.82030 (n, π^*) 0.34615 (n, π^*) -0.20272 (n, π^*, π, π^*)	-0.83819 (n, π^*) 0.31314 (n, π^*) 0.20367 (n, π^*, π, π^*)
T1	-0.87318 (π, π^*) -0.29684 (π, π^*)	0.86792 (π, π^*) 0.31588 (π, π^*)	0.85174 (π, π^*) 0.35469 (π, π^*)	0.84648 (π, π^*) 0.36799 (π, π^*)
T2	0.84079 (n, π^*) 0.33093 (n, π^*)	0.81708 (π, π^*) 0.46566 (π, π^*)	0.83284 (n, π^*) 0.36186 (n, π^*) 0.15729 (n, π^*, π, π^*)	-0.80587 (π, π^*) -0.48577 (π, π^*)
T3	0.68885 (π, π^*) 0.61577 (π, π^*)	-0.82294 (n, π^*) 0.34977 (n, π^*) -0.22141 (n, π^*, π, π^*)	-0.68924 (π, π^*) -0.61980 (π, π^*)	0.80445 (n, π^*) -0.40149 (n, π^*) 0.18997 (n, π^*, π, π^*)

II.

The molecular geometries corresponding to MECIs between S_0 and S_1 for **1** and **2** are listed below along with gradient difference and derivative coupling vectors that define the branching plane. At these geometries, S_0 and S_1 are effectively degenerate at the MS-CASPT2 level.

MECI **1** – S_0 = -489.5178447 Hartree, S_1 = -489.5177926 Hartree

MECI **2** – S_0 = -489.5246769 Hartree, S_1 = -489.5246080 Hartree

Geometry of MECI 1

C	-1.586340	0.609281	-0.357904
C	0.011098	0.633329	-0.257813
C	0.306673	1.903256	-0.200924
C	-0.860153	4.006070	-0.139189
C	-2.311214	4.181567	-0.073169
C	-2.860036	2.924863	-0.239598
H	0.603663	-0.220534	0.012792
H	-2.839864	5.092203	0.146040
H	-3.896941	2.635090	-0.212573
H	-2.137252	0.151193	0.467010
O	0.169950	4.633952	0.053310
O	1.381859	2.827090	0.136992
N	-1.893418	2.004438	-0.554382
N	-0.738203	2.717206	-0.493958

Gradient difference vector (Hartree/bohr)

C	0.213717	0.123679	0.043577
C	-0.324036	-0.247153	0.065748
C	0.383789	0.564276	0.086644
C	0.078298	0.098372	0.012566
C	-0.010131	-0.033501	0.020086
C	-0.040504	0.025302	-0.001929
H	0.002310	-0.002436	-0.008758
H	-0.002388	-0.000227	-0.000111
H	-0.001042	0.000797	-0.002710
H	-0.003552	-0.042128	-0.049567
O	-0.177377	0.112615	0.021428
O	-0.096447	-0.410364	-0.105982
N	0.022462	-0.043088	0.017466
N	-0.045100	-0.146145	-0.098459

Derivative coupling vector (Hartree/bohr)

C	0.033982	-0.001419	-0.156813
C	-0.288540	0.055255	0.375656
C	0.035842	-0.030846	0.265165

C	-0.245565	-0.055166	0.010070
C	0.132860	-0.035364	0.097056
C	0.001542	-0.059236	-0.099678
H	-0.001555	0.003220	-0.009478
H	-0.001231	0.002067	-0.006241
H	0.001006	-0.000287	-0.004946
H	0.051358	-0.048729	-0.025900
O	0.167428	-0.216209	0.245682
O	0.184363	0.291092	-0.393190
N	0.087152	0.141156	0.018047
N	-0.158716	-0.045629	-0.315637

Geometry of MECI 2

C	-1.382793	0.757724	-0.061049
C	-0.128631	0.622643	-0.354693
C	0.495829	1.961876	0.076805
C	-0.914925	4.051427	0.182323
C	-2.343477	4.086456	-0.210227
C	-2.804050	2.820601	-0.195181
O	-0.095883	4.918841	0.143650
O	-2.611845	0.183519	0.457497
H	0.430013	-0.289917	-0.468631
H	-2.866872	4.975768	-0.515818
H	-3.770444	2.404286	-0.414403
H	1.180831	2.533763	-0.537569
N	-0.644671	2.722790	0.548523
N	-1.784181	1.983103	0.338266

Gradient difference vector (Hartree/bohr)

C	-0.691769	-0.103613	0.249832
C	0.354872	0.181362	0.038082
C	-0.228119	-0.140358	-0.090909
C	0.010975	0.024996	-0.002516
C	-0.007240	-0.006732	-0.001014
C	0.100996	-0.021524	0.059989

O	0.004147	0.007772	0.001742
O	0.206602	-0.158872	-0.133096
H	0.002209	0.000762	-0.029904
H	-0.000023	0.001195	0.003632
H	0.002629	-0.012162	-0.007614
H	0.046248	-0.012351	0.060178
N	0.009707	0.011097	-0.097770
N	0.188765	0.228429	-0.050633

Derivative coupling vector (Hartree/bohr)

C	0.044913	0.099773	-0.007277
C	0.105583	-0.200813	0.232056
C	-0.109593	0.126551	-0.148027
C	-0.061469	-0.066915	-0.106850
C	0.095598	0.018754	0.031556
C	-0.022796	-0.084557	-0.036898
O	0.096387	0.085994	0.026183
O	-0.061232	-0.401850	-0.210545
H	-0.013829	-0.003711	-0.026142
H	0.005673	0.002674	0.001671
H	-0.002929	0.024271	0.023374
H	0.018647	-0.012079	-0.058851
N	0.408232	0.211501	0.053046
N	-0.504710	0.200589	0.226697

III.

In Table S2, we list absolute values of spin-orbit matrix elements used for calculating the rate of ISC from S_1 to various triplet sublevels in **1-4**

Table S2. Absolute values of spin-orbit matrix elements ($\langle \phi_{S_1} | \hat{H}_{SO} | \phi_{T_n}(M_s) \rangle, s = 0, \pm 1$) in cm^{-1} between S_1 and sublevels of T_n for **1-4** at the Franck-Condon geometry.

	1	2	3	4
$S_1-T_1 (M_{s=0})$	0.0	2.9	0.0	4.6
$S_1-T_1 (M_{s=1})$	6.1	0.1	2.8	0.3
$S_1-T_1 (M_{s=-1})$	6.1	0.1	2.8	0.3

$S_1-T_2 (M_{S=0})$	1.0	0.3	1.0	1.6
$S_1-T_2 (M_{S=1})$	12.2	12.7	5.4	15.6
$S_1-T_2 (M_{S=-1})$	12.2	12.7	5.4	15.6
$S_1-T_3 (M_{S=0})$	2.4	0.3	2.4	0.7
$S_1-T_3 (M_{S=1})$	16.1	14.7	15.3	7.4
$S_1-T_3 (M_{S=-1})$	16.1	14.7	15.3	7.4
