Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

First-principle methods for calculating rate constants of internal-conversion and intersystem-crossing transitions

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Table S_1. The nonzero matrix elements (in cm^{-1}) of one-electronic spin-orbital coupling interaction operator between S_1 and energy lower triplets states (T_n).

	Compounds					
State	PM567	PSO	1B3N	H_2P	Alq_3	$Ir(ppy)_3$
$<\psi(S_1)\|H_{SO}\|\psi(T_1)>$	0.6	1.5	-	1.6	0.45	110
$<\psi(S_1)\|H_{SO}\|\psi(T_2)>$	0.3	0.5	-	-	-	-
$<\psi(S_1)\|H_{SO}\|\psi(T_3)>$	-	-	0.1	-	-	-
$<\psi(S_1)\|H_{SO}\|\psi(T_4)>$	-	-	1.2	-	-	-

	Compounds				
	Naphthalene	Anthracene	Tetracene	Pentacene	Hexacene
$<\psi(S_1)\|H_{SO}\|\psi(T_1)>$	2.47	2.5	2.2	2.2	2.2

The Cartesian coordinates (in Angstrom) of atoms of equilibrium geometries of S_0 and S_1 states of considered compounds

2.1. PM567

	S_0			S_1		
	X	Y	Z	X	Y	Z
C	1.2168	0.8302	-0.1620	1.2348	0.8686	-0.2179
N	1.2443	-0.5659	-0.1513	1.2604	-0.5442	-0.2755
B	0.0082	-1.5062	-0.0850	-0.0038	-1.4677	-0.2332
N	-1.2293	-0.5810	0.0853	-1.1962	-0.5526	0.0579
C	-1.2213	0.8153	0.0620	-1.2163	0.8595	0.0133
C	-0.0105	1.5181	-0.0963	-0.0563	1.5885	-0.1993
C	-2.4947	-1.0097	0.2502	-2.4585	-1.0045	0.2803
C	-3.3629	0.1045	0.3627	-3.3371	0.0966	0.4082
C	-2.5750	1.2546	0.2416	-2.5843	1.2655	0.2419
C	2.5763	1.2848	-0.2264	2.5286	1.2985	-0.1724
C	3.3847	0.1441	-0.2667	3.3968	0.0646	-0.2512
C	2.5228	-0.9801	-0.2216	2.5442	-1.0212	-0.3089
C	-3.1055	2.6569	0.3346	-3.1201	2.6610	0.3637
C	3.0999	2.6931	-0.2129	3.1255	2.6614	-0.0611
C	2.8792	-2.4315	-0.2445	2.8524	-2.4831	-0.3939
C	-2.8316	-2.4655	0.2890	-2.7694	-2.4632	0.3353
C	-5.6497	0.0415	-0.7641	-5.6621	0.0344	-0.6317
C	-4.8541	0.0312	0.5540	-4.8175	0.0020	0.6561
C	5.5441	-0.0058	1.0810	5.4647	0.0263	1.2152
C	4.8885	0.0844	-0.3093	4.8846	0.0594	-0.2220
C	-0.0290	3.0231	-0.1996	-0.0588	3.0666	-0.4658
F	-0.1019	-2.2473	-1.2614	-0.1237	-2.1195	-1.4616
F	0.1225	-2.3569	1.0153	0.1705	-2.3999	0.7932
H	-2.5421	3.2718	1.0427	-2.4907	3.2936	0.9984
H	-4.1459	2.6468	0.6677	-4.1197	2.6487	0.8069
H	-3.0883	3.1755	-0.6322	-3.2137	3.1694	-0.6057
H	2.6741	3.2873	0.6012	2.3959	3.4283	0.1862
H	4.1841	2.6942	-0.0805	3.9056	2.6762	0.7101
H	2.8925	3.2282	-1.1483	3.6184	2.9541	-0.9991
H	2.3219	-2.9447	-1.0336	2.2998	-2.9439	-1.2178
H	3.9487	-2.5717	-0.4097	3.9215	-2.6387	-0.5570
H	2.5978	-2.9096	0.6986	2.5535	-3.0054	0.5192
H	-3.8977	-2.6200	0.4624	-3.8329	-2.6318	0.5128
H	-2.5521	-2.9433	-0.6553	-2.4891	-2.9516	-0.6056
H	-2.2591	-2.9681	1.0735	-2.1903	-2.9577	1.1218
H	-6.7268	-0.0180	-0.5742	-6.7309	-0.0367	-0.4026
H	-5.3697	-0.8054	-1.3985	-5.3995	-0.7970	-1.2932
H	-5.4558	0.9562	-1.3336	-5.4949	0.9624	-1.1877
H	-5.1884	0.8664	1.1810	-5.1350	0.8222	1.3115

H	-5.1062	-0.8744	1.1174	-5.0401	-0.9184	1.2075
H	6.6353	-0.0539	0.9995	6.5585	0.0307	1.1791
H	5.2046	-0.8970	1.6181	5.1382	-0.8739	1.7424
H	5.2872	0.8639	1.6943	5.1382	0.8925	1.7980
H	5.2020	-0.7785	-0.9088	5.2612	-0.8116	-0.7689
H	5.2795	0.9619	-0.8364	5.2712	0.9485	-0.7352
H	-0.9499	3.3767	-0.6573	-1.0364	3.4111	-0.7975
H	0.7972	3.3883	-0.8050	0.6537	3.3170	-1.2596
H	0.0513	3.4932	0.7887	0.2152	3.6724	0.4118

2.2. Psoralene

	S_0			S_1		
	X	Y	Z	X	Y	Z
O	-4.0462	0.9830	0.0000	-4.0508	1.0685	-0.0190
C	-3.0235	0.3519	0.0000	-3.1107	0.3144	-0.0056
O	-1.8211	1.0623	0.0000	-1.7653	1.0847	0.0176
C	-2.9044	-1.0991	0.0000	-2.9708	-1.0831	-0.0071
C	-1.7038	-1.7094	0.0000	-1.7363	-1.7396	0.0025
C	-0.4799	-0.9533	0.0000	-0.5104	-0.9813	0.0031
C	-0.5961	0.4587	0.0000	-0.5997	0.4590	0.0059
C	0.5131	1.2943	0.0000	0.5537	1.2953	-0.0001
C	0.7877	-1.5477	0.0000	0.7555	-1.5538	0.0002
C	1.9150	-0.7362	0.0000	1.9274	-0.7314	-0.0020
C	1.7419	0.6637	0.0000	1.7788	0.6621	-0.0026
O	2.9546	1.2860	0.0000	3.0291	1.2716	-0.0058
C	3.3434	-0.9441	0.0000	3.3214	-0.9732	-0.0051
C	3.9012	0.2836	0.0000	3.9296	0.2785	-0.0063
H	-3.8368	-1.6455	0.0000	-3.9014	-1.6374	-0.0164
H	-1.6412	-2.7924	0.0000	-1.6848	-2.8211	0.0019
H	0.8715	-2.6281	0.0000	0.8558	-2.6350	0.0000
H	0.4019	2.3695	0.0000	0.4311	2.3712	-0.0000
H	3.8716	-1.8835	0.0000	3.8382	-1.9223	-0.0057
H	4.9229	0.6228	0.0000	4.9682	0.5737	-0.0087

2.3. 4B

	S_0			S_1		
	X	Y	Z	X	Y	Z
O	3.8808	-0.0478	0.0000	3.8946	-0.0480	0.0000
C	3.0338	-1.1443	0.0000	3.0514	-1.1470	0.0000
C	1.6942	-0.7367	0.0000	1.6963	-0.7180	0.0000
C	0.6947	-1.7121	0.0000	0.6760	-1.7137	0.0000
C	1.0692	-3.0614	0.0000	1.0715	-3.0791	0.0000
O	-0.0478	-3.8808	0.0000	-0.0480	-3.8946	0.0000
C	-1.1443	-3.0339	0.0000	-1.1470	-3.0514	0.0000
C	-0.7367	-1.6943	0.0000	-0.7180	-1.6963	0.0000
C	-1.7121	-0.6947	0.0000	-1.7137	-0.6760	0.0000
C	-3.0614	-1.0692	0.0000	-3.0791	-1.0715	0.0000
O	-3.8808	0.0478	0.0000	-3.8946	0.0480	0.0000
C	-3.0338	1.1443	0.0000	-3.0514	1.1470	0.0000
C	-1.6942	0.7367	0.0000	-1.6963	0.7180	0.0000
C	-0.6947	1.7121	0.0000	-0.6760	1.7137	0.0000

C	-1.0692	3.0614	0.0000	-1.0715	3.0791	0.0000
C	1.1443	3.0338	0.0000	1.1470	3.0514	0.0000
C	0.7367	1.6942	0.0000	0.7180	1.6963	0.0000
C	1.7121	0.6947	0.0000	1.7137	0.6760	0.0000
C	3.0614	1.0692	0.0000	3.0791	1.0715	0.0000
C	3.4726	2.4082	0.0000	3.4785	2.3920	0.0000
C	2.4930	3.4121	0.0000	2.4769	3.4185	0.0000
H	2.7760	4.4588	0.0000	2.7685	4.4623	0.0000
C	-2.4082	3.4726	0.0000	-2.3920	3.4785	0.0000
C	-3.4121	2.4930	0.0000	-3.4185	2.4769	0.0000
H	-2.6656	4.5259	0.0000	-2.6579	4.5293	0.0000
C	-3.4726	-2.4082	0.0000	-3.4785	-2.3920	0.0000
C	-2.4930	-3.4121	0.0000	-2.4769	-3.4185	0.0000
H	-4.5259	-2.6656	0.0000	-4.5292	-2.6579	0.0000
C	2.4082	-3.4726	0.0000	2.3920	-3.4786	0.0000
C	3.4121	-2.4930	0.0000	3.4185	-2.4769	0.0000
H	4.4588	-2.7760	0.0000	4.4623	-2.7685	0.0000
O	0.0478	3.8808	0.0000	0.0480	3.8946	0.0000
H	4.5259	2.6656	0.0000	4.5292	2.6579	0.0000
H	-4.4588	2.7760	0.0000	-4.4623	2.7685	0.0000
H	-2.7760	-4.4588	0.0000	-2.7685	-4.4623	0.0000
H	2.6656	-4.5259	0.0000	2.6579	-4.5293	0.0000

2.4. AOC

	S_0			S_1		
	X	Y	Z	X	Y	Z
C	1.7104	-0.2362	0.0000	1.7106	-0.2487	0.0000
C	0.7143	0.7681	0.0000	0.7017	0.7693	0.0000
C	1.7044	-1.6695	0.0000	1.7067	-1.6488	0.0000
C	0.7168	-2.6687	0.0000	0.6992	-2.6697	0.0000
C	-0.7168	-2.6687	0.0000	-0.6992	-2.6697	0.0000
C	-1.7044	-1.6695	0.0000	-1.7067	-1.6488	0.0000
C	-1.7104	-0.2362	0.0000	-1.7106	-0.2487	0.0000
C	-0.7143	0.7681	0.0000	-0.7017	0.7693	0.0000
C	3.0423	0.1524	0.0000	3.0628	0.1587	0.0000
C	3.4765	1.5092	0.0000	3.4832	1.4962	0.0000
C	2.4581	2.5335	0.0000	2.4477	2.5329	0.0000
C	1.1024	2.1005	0.0000	1.1065	2.1109	0.0000
O	0.0000	2.9316	0.0000	0.0000	2.9397	0.0000
C	-1.1024	2.1005	0.0000	-1.1065	2.1109	0.0000
C	-2.4581	2.5335	0.0000	-2.4477	2.5329	0.0000
C	-3.0423	0.1524	0.0000	-3.0628	0.1587	0.0000
C	3.0535	-2.0525	0.0000	3.0678	-2.0522	0.0000
O	3.8802	-0.9417	0.0000	3.8936	-0.9400	0.0000
C	3.4735	-3.3863	0.0000	3.4757	-3.3693	0.0000
C	2.4971	-4.3854	0.0000	2.4807	-4.3934	0.0000
C	1.1373	-4.0222	0.0000	1.1397	-4.0406	0.0000
N	-0.0000	-4.8226	0.0000	-0.0000	-4.8365	0.0000
C	-1.1373	-4.0222	0.0000	-1.1397	-4.0406	0.0000
C	-2.4971	-4.3854	0.0000	-2.4807	-4.3934	0.0000
C	-3.4735	-3.3863	0.0000	-3.4757	-3.3693	0.0000

C	-3.0535	-2.0525	0.0000	-3.0678	-2.0522	0.0000
O	-3.8802	-0.9417	0.0000	-3.8936	-0.9400	0.0000
C	-3.4765	1.5092	0.0000	-3.4832	1.4962	0.0000
C	-2.8520	3.8913	0.0000	-2.8530	3.8946	0.0000
C	-4.8364	1.8958	0.0000	-4.8507	1.8958	0.0000
C	4.8364	1.8958	0.0000	4.8507	1.8958	0.0000
C	2.8520	3.8913	0.0000	2.8530	3.8946	0.0000
C	-4.1904	4.2335	0.0000	-4.1854	4.2328	0.0000
C	-5.1865	3.2322	0.0000	-5.1942	3.2247	0.0000
H	4.5284	-3.6375	0.0000	4.5287	-3.6272	0.0000
H	2.7916	-5.4305	0.0000	2.7858	-5.4347	0.0000
H	-2.0831	4.6575	0.0000	-2.0859	4.6627	0.0000
H	-5.5977	1.1220	0.0000	-5.6139	1.1238	0.0000
H	-4.4790	5.2805	0.0000	-4.4759	5.2792	0.0000
H	-6.2350	3.5153	0.0000	-6.2408	3.5139	0.0000
C	4.1904	4.2335	0.0000	4.1854	4.2328	0.0000
C	5.1865	3.2322	0.0000	5.1942	3.2247	0.0000
H	-2.7916	-5.4305	0.0000	-2.7858	-5.4347	0.0000
H	-4.5284	-3.6375	0.0000	-4.5287	-3.6272	0.0000
H	5.5977	1.1220	0.0000	5.6139	1.1238	0.0000
H	2.0831	4.6575	0.0000	2.0859	4.6627	0.0000
H	4.4790	5.2805	0.0000	4.4759	5.2792	0.0000
H	6.2350	3.5153	0.0000	6.2408	3.5139	0.0000
H	-0.0000	-5.8293	0.0000	-0.0000	-5.8432	0.0000

2.5. 1B3N

	S_0			S_1		
	X	Y	Z	X	Y	Z
C	0.6995	-2.3083	0.0000	0.7069	-2.2931	0.0000
C	-0.6995	-2.3083	0.0000	-0.7069	-2.2931	0.0000
C	1.7169	-1.3035	0.0000	1.7073	-1.3011	0.0000
C	1.7186	0.1105	0.0000	1.7110	0.1140	0.0000
C	0.7076	1.1213	0.0000	0.7096	1.1172	0.0000
C	-0.7076	1.1213	0.0000	-0.7096	1.1172	0.0000
C	-1.7186	0.1105	0.0000	-1.7110	0.1140	0.0000
C	-1.7169	-1.3035	0.0000	-1.7073	-1.3011	0.0000
C	1.3679	-3.5410	0.0000	1.3705	-3.5415	0.0000
C	0.7014	-4.7714	0.0000	0.7161	-4.7588	0.0000
C	-0.7014	-4.7714	0.0000	-0.7161	-4.7588	0.0000
C	-1.3679	-3.5410	0.0000	-1.3705	-3.5415	0.0000
O	-2.7385	-3.3456	0.0000	-2.7505	-3.3406	0.0000
C	-2.9287	-1.9768	0.0000	-2.9453	-1.9817	0.0000
C	-4.1956	-1.3253	0.0000	-4.2019	-1.3347	0.0000
C	-2.9354	0.7768	0.0000	-2.9433	0.7781	0.0000
C	2.9287	-1.9768	0.0000	2.9453	-1.9817	0.0000
O	2.7385	-3.3456	0.0000	2.7505	-3.3406	0.0000
C	4.1956	-1.3253	0.0000	4.2019	-1.3347	0.0000
C	4.1993	0.1211	0.0000	4.2031	0.1245	0.0000
C	2.9354	0.7768	0.0000	2.9433	0.7781	0.0000
O	2.7429	2.1446	0.0000	2.7513	2.1399	0.0000
C	1.3754	2.3374	0.0000	1.3746	2.3429	0.0000

C	0.7230	3.6036	0.0000	0.7303	3.5995	0.0000
C	-0.7230	3.6036	0.0000	-0.7303	3.5995	0.0000
C	-1.3754	2.3374	0.0000	-1.3746	2.3429	0.0000
O	-2.7429	2.1446	0.0000	-2.7513	2.1399	0.0000
C	-4.1993	0.1211	0.0000	-4.2031	0.1245	0.0000
C	-5.4310	-2.0131	0.0000	-5.4414	-2.0199	0.0000
C	5.4310	-2.0131	0.0000	5.4414	-2.0199	0.0000
C	5.4390	0.8015	0.0000	5.4436	0.7985	0.0000
C	1.4072	4.8410	0.0000	1.4109	4.8447	0.0000
C	-1.4072	4.8410	0.0000	-1.4109	4.8447	0.0000
C	-5.4390	0.8015	0.0000	-5.4436	0.7985	0.0000
C	-6.6234	-1.3158	0.0000	-6.6361	-1.3224	0.0000
C	-6.6270	0.0967	0.0000	-6.6362	0.0918	0.0000
C	6.6234	-1.3158	0.0000	6.6361	-1.3224	0.0000
C	6.6270	0.0967	0.0000	6.6362	0.0918	0.0000
C	0.7062	6.0313	0.0000	0.7107	6.0303	0.0000
C	-0.7062	6.0313	0.0000	-0.7107	6.0303	0.0000
H	-5.4232	-3.0992	0.0000	-5.4355	-3.1062	0.0000
H	5.4232	-3.0992	0.0000	5.4355	-3.1062	0.0000
H	5.4384	1.8877	0.0000	5.4472	1.8847	0.0000
H	2.4933	4.8369	0.0000	2.4973	4.8431	0.0000
H	-2.4933	4.8369	0.0000	-2.4973	4.8431	0.0000
H	-5.4384	1.8877	0.0000	-5.4472	1.8847	0.0000
H	-7.5660	-1.8565	0.0000	-7.5784	-1.8628	0.0000
H	-7.5726	0.6323	0.0000	-7.5801	0.6300	0.0000
H	7.5660	-1.8565	0.0000	7.5784	-1.8628	0.0000
H	7.5726	0.6323	0.0000	7.5801	0.6300	0.0000
H	1.2444	6.9754	0.0000	1.2469	6.9754	0.0000
H	-1.2444	6.9754	0.0000	-1.2469	6.9754	0.0000
H	1.2548	-5.7045	0.0000	1.2641	-5.6944	0.0000
H	-1.2548	-5.7045	0.0000	-1.2641	-5.6944	0.0000

2.6. H_2P

	S_0			S_1		
X	Y		Z	X	Y	Z
C	2.8963	-1.130	0.0000	2.8973	-1.1331	0.0000
N	2.1175	0.000	0.0000	2.1154	0.0000	0.0000
C	2.8963	1.130	0.0000	2.8973	1.1331	0.0000
C	0.6782	-4.259	0.0000	0.6814	-4.2780	0.0000
C	-0.6782	-4.259	0.0000	-0.6814	-4.2780	0.0000
C	-1.0849	-2.856	0.0000	-1.0891	-2.8826	0.0000
N	-0.0000	-2.030	0.0000	0.0000	-2.0516	0.0000
C	1.0849	-2.856	0.0000	1.0891	-2.8827	0.0000
C	-0.6782	4.259	0.0000	-0.6814	4.2780	0.0000
C	0.6782	4.259	0.0000	0.6814	4.2780	0.0000
C	1.0849	2.856	0.0000	1.0891	2.8826	0.0000
N	-0.0000	2.030	0.0000	0.0000	2.0516	0.0000
C	-1.0849	2.856	0.0000	-1.0891	2.8826	0.0000
C	-4.2610	-0.686	0.0000	-4.2620	-0.6875	0.0000
C	-4.2610	0.686	0.0000	-4.2620	0.6875	0.0000
C	-2.8963	1.130	0.0000	-2.8973	1.1331	0.0000

N	-2.1175	0.000	0.0000	-2.1154	-0.0000	0.0000
C	-2.8963	-1.130	0.0000	-2.8973	-1.1331	0.0000
C	4.2610	0.686	0.0000	4.2620	0.6875	0.0000
C	4.2610	-0.686	0.0000	4.2620	-0.6875	0.0000
C	2.4222	-2.441	0.0000	2.4283	-2.4489	0.0000
C	-2.4222	2.441	0.0000	-2.4283	2.4489	0.0000
C	-2.4222	-2.441	0.0000	-2.4283	-2.4489	0.0000
C	2.4222	2.441	0.0000	2.4283	2.4489	0.0000
H	1.1019	0.000	0.0000	1.1012	0.0000	0.0000
H	1.3524	-5.107	0.0000	1.3535	-5.1277	0.0000
H	-1.3524	-5.107	0.0000	-1.3535	-5.1277	0.0000
H	-1.3524	5.107	0.0000	-1.3535	5.1277	0.0000
H	1.3524	5.107	0.0000	1.3535	5.1277	0.0000
H	-5.1177	-1.347	0.0000	-5.1191	-1.3483	0.0000
H	-5.1177	1.347	0.0000	-5.1191	1.3483	0.0000
H	-1.1019	-0.000	0.0000	-1.1012	-0.0000	0.0000
H	5.1177	1.347	0.0000	5.1191	1.3483	0.0000
H	5.1177	-1.347	0.0000	5.1191	-1.3483	0.0000
H	3.1800	-3.220	0.0000	3.1919	-3.2220	0.0000
H	-3.1800	3.220	0.0000	-3.1919	3.2220	0.0000
H	-3.1800	-3.220	0.0000	-3.1919	-3.2220	0.0000
H	3.1800	3.220	0.0000	3.1919	3.2220	0.0000

2.7. Alq_3

	S_0			S_1	
X	Y	Z	X	Y	Z
C 4.3840	-2.8643	-1.2294	4.3968	-2.8899	-1.2575
C 5.0076	-2.0122	-0.3354	4.9753	-1.9844	-0.3544
C 4.2423	-1.0042	0.3003	4.2187	-0.9631	0.3011
C 2.8554	-0.9080	-0.0088	2.8659	-0.8953	0.0116
C 2.2149	-1.7958	-0.9403	2.2553	-1.8126	-0.9158
C 3.0109	-2.7715	-1.5383	3.0510	-2.8200	-1.5472
C 4.7420	-0.0643	1.2356	4.7685	-0.0257	1.2202
C 3.8983	0.8733	1.7938	3.8697	0.9163	1.7688
C 2.5380	0.8881	1.4263	2.5400	0.9186	1.4339
C -4.0904	-3.1332	0.8076	-4.1275	-3.0257	0.8042
C -3.5818	-2.2765	-0.2006	-3.5802	-2.1809	-0.1921
C -2.3204	-1.6576	0.0155	-2.2981	-1.6340	0.0249
C -4.2202	-1.9735	-1.4301	-4.2085	-1.8264	-1.4106
C -3.6163	-1.1262	-2.3373	-3.5695	-0.9968	-2.3014
C -1.5461	-1.8750	1.2056	-1.5333	-1.9008	1.2072
C -0.0099	2.2623	-1.3367	-0.0183	2.1854	-1.3393
C 0.0968	3.3299	-2.2265	0.0665	3.2426	-2.2334
C -0.3033	4.6265	-1.8357	-0.3487	4.5352	-1.8512
C -0.8120	4.9084	-0.5799	-0.8526	4.8196	-0.6013
C -0.9371	3.8570	0.3617	-0.9582	3.7737	0.3463
C -0.5300	2.5515	-0.0303	-0.5402	2.4802	-0.0355
C -1.4384	3.9800	1.6825	-1.4539	3.9022	1.6667
C -1.5076	2.8728	2.5045	-1.5071	2.8073	2.4971
C -1.0746	1.6187	2.0244	-1.0628	1.5575	2.0258
C -2.3613	-0.5599	-2.0328	-2.2877	-0.5019	-1.9930
C -2.0871	-2.7270	2.1658	-2.1082	-2.7314	2.1563

C	-3.3429	-3.3381	1.9532	-3.3909	-3.2795	1.9392
H	4.9705	-3.6385	-1.7173	5.0178	-3.6453	-1.7260
H	6.0662	-2.1045	-0.1147	6.0373	-2.0575	-0.1412
H	2.5552	-3.4563	-2.2453	2.5651	-3.4982	-2.2388
H	5.7940	-0.0912	1.5077	5.8197	-0.0377	1.4757
H	4.2621	1.6004	2.5117	4.2251	1.6608	2.4733
H	1.8505	1.6114	1.8511	1.8511	1.6420	1.8537
H	0.4905	3.1492	-3.2211	0.4626	3.0613	-3.2263
H	-0.2059	5.4333	-2.5575	-0.2652	5.3360	-2.5803
H	-1.1138	5.9152	-0.3092	-1.1644	5.8240	-0.3356
H	-1.7673	4.9525	2.0398	-1.7913	4.8740	2.0164
H	-1.8896	2.9502	3.5166	-1.8847	2.8903	3.5094
H	-1.1041	0.7218	2.6334	-1.0733	0.6629	2.6396
H	-1.5266	-2.9196	3.0745	-1.5571	-2.9579	3.0623
H	-3.7304	-3.9983	2.7247	-3.8066	-3.9301	2.7033
H	-5.0508	-3.6194	0.6691	-5.1102	-3.4626	0.6618
H	-5.1870	-2.4182	-1.6520	-5.1971	-2.2184	-1.6329
H	-4.0898	-0.8898	-3.2839	-4.0349	-0.7173	-3.2393
H	-1.8422	0.1032	-2.7163	-1.7372	0.1517	-2.6607
N	2.0363	0.0261	0.5530	1.9935	0.0142	0.5487
N	-0.6005	1.4716	0.7938	-0.5974	1.4123	0.8002
N	-1.7453	-0.8191	-0.8886	-1.6828	-0.8148	-0.8643
O	0.9328	-1.6261	-1.1619	1.0071	-1.6865	-1.1440
O	-0.3928	-1.2465	1.3017	-0.3575	-1.3310	1.2993
O	0.3167	1.0158	-1.5911	0.3221	0.9470	-1.5855
Al	0.1206	-0.2525	-0.2149	0.1762	-0.2493	-0.1387

2.8. $Ir(ppy)_3$

	S_0			S_1		
	X	Y	Z	X	Y	Z
Ir	-0.004	0.0011	-0.0121	0.0262	0.0112	-0.0906
N	-0.610	-1.7752	1.0629	-0.5529	-1.7565	1.0616
C	0.027	-2.3122	2.1110	0.1328	-2.2590	2.0950
C	-0.397	-3.4745	2.7292	-0.2596	-3.4171	2.7416
C	-1.532	-4.1070	2.2243	-1.4041	-4.0678	2.2838
C	-2.186	-3.5599	1.1345	-2.1049	-3.5484	1.2081
C	-1.710	-2.3790	0.5509	-1.6605	-2.3741	0.5897
C	-2.302	-1.7041	-0.6103	-2.2981	-1.7206	-0.5654
C	-1.630	-0.5417	-1.0676	-1.6606	-0.5639	-1.0752
C	-2.180	0.0985	-2.1910	-2.2682	0.0713	-2.1665
C	-3.321	-0.3815	-2.8213	-3.4397	-0.4182	-2.7338
C	-3.967	-1.5272	-2.3516	-4.0513	-1.5620	-2.2200
C	-3.454	-2.1849	-1.2463	-3.4805	-2.2088	-1.1356
H	-3.958	-3.0770	-0.8847	-3.9649	-3.0970	-0.7402
H	-4.859	-1.9002	-2.8447	-4.9649	-1.9445	-2.6636
H	-3.715	0.1384	-3.6907	-3.8811	0.0917	-3.5857
H	-1.694	0.9886	-2.5795	-1.8057	0.9604	-2.5853
H	-3.063	-4.0471	0.7265	-2.9889	-4.0538	0.8401
H	-1.900	-5.0227	2.6762	-1.7447	-4.9811	2.7613
H	0.148	-3.8732	3.5756	0.3188	-3.7993	3.5737
H	0.908	-1.7766	2.4474	1.0158	-1.6974	2.3828
C	1.305	-1.1277	-1.0442	1.2829	-1.1225	-1.1036

C	1.052	-1.9036	-2.1874	0.9938	-1.8989	-2.2374
C	2.052	-2.6461	-2.8030	1.9801	-2.6325	-2.8840
C	3.353	-2.6482	-2.2962	3.2917	-2.6158	-2.3809
C	3.640	-1.8937	-1.1710	3.6155	-1.8813	-1.2527
C	2.634	-1.1394	-0.5512	2.6332	-1.1252	-0.5826
C	2.895	-0.3003	0.6247	2.8618	-0.3519	0.6011
N	1.811	0.3530	1.1078	1.7231	0.3106	1.0947
C	1.927	1.1693	2.1629	1.8701	1.1683	2.1393
C	3.128	1.3756	2.8179	3.0507	1.3525	2.7993
C	4.255	0.7060	2.3443	4.2057	0.6313	2.3638
C	4.138	-0.1296	1.2473	4.0916	-0.1924	1.2731
H	5.010	-0.6452	0.8629	4.9607	-0.7309	0.9090
H	5.219	0.8415	2.8252	5.1550	0.7481	2.8740
H	3.177	2.0467	3.6670	3.0993	2.0433	3.6330
H	1.015	1.6667	2.4742	0.9705	1.6996	2.4359
H	4.654	-1.8957	-0.7811	4.6383	-1.8955	-0.8882
H	4.132	-3.2304	-2.7777	4.0668	-3.1895	-2.8817
H	1.819	-3.2302	-3.6898	1.7430	-3.2108	-3.7713
H	0.050	-1.9150	-2.6054	-0.0188	-1.9028	-2.6289
N	-1.247	1.3951	1.0799	-1.2799	1.3911	1.0072
C	-2.043	1.0857	2.1114	-2.1328	1.0570	1.9824
C	-2.849	2.0184	2.7383	-2.9814	1.9758	2.5725
C	-2.828	3.3278	2.2605	-2.9400	3.2928	2.1179
C	-2.014	3.6470	1.1878	-2.0668	3.6351	1.1003
C	-1.217	2.6600	0.5940	-1.2324	2.6598	0.5421
C	-0.323	2.8585	-0.5533	-0.2796	2.8765	-0.5541
C	0.346	1.7032	-1.0290	0.4221	1.7356	-1.0164
C	1.186	1.8778	-2.1414	1.3562	1.9225	-2.0481
C	1.353	3.1180	-2.7440	1.5705	3.1758	-2.6052
C	0.687	4.2437	-2.2554	0.8696	4.2894	-2.1402
C	-0.150	4.1098	-1.1609	-0.0498	4.1381	-1.1138
H	-0.667	4.9882	-0.7841	-0.5790	5.0129	-0.7484
H	0.821	5.2124	-2.7262	1.0433	5.2685	-2.5746
H	2.011	3.2136	-3.6045	2.2951	3.2901	-3.4063
H	1.712	1.0175	-2.5439	1.9055	1.0656	-2.4226
H	-1.999	4.6576	0.7986	-2.0335	4.6520	0.7297
H	-3.449	4.0911	2.7188	-3.5916	4.0447	2.5511
H	-3.479	1.7240	3.5691	-3.6566	1.6662	3.3609
H	-2.020	0.0473	2.4259	-2.1195	0.0153	2.2851

2.9. Naphthalene

	S_0			S_1		
	X	Y	Z	X	Y	Z
H	-1.2424	-2.4903	0.0000	-1.2496	-2.5038	0.0000
C	-1.2448	-1.4028	0.0000	-1.2445	-1.4167	0.0000
C	-2.4335	-0.7086	0.0000	-2.4569	-0.7137	0.0000
C	-2.4335	0.7086	0.0000	-2.4569	0.7137	0.0000
C	-1.2448	1.4028	0.0000	-1.2445	1.4167	0.0000
C	-0.0000	0.7171	0.0000	-0.0000	0.7447	0.0000
C	-0.0000	-0.7171	0.0000	-0.0000	-0.7447	0.0000

C	1.2448	-1.4028	0.0000		1.2445	-1.4167	0.0000
C	2.4335	-0.7086	0.0000		2.4569	-0.7137	0.0000
C	2.4335	0.7086	0.0000		2.4569	0.7137	0.0000
C	1.2448	1.4028	0.0000		1.2445	1.4167	0.0000
H	-3.3781	-1.2452	0.0000		-3.3978	-1.2539	0.0000
H	-3.3781	1.2452	0.0000		-3.3978	1.2539	0.0000
H	-1.2424	2.4903	0.0000		-1.2496	2.5038	0.0000
H	1.2424	2.4903	0.0000		1.2496	2.5038	0.0000
H	3.3781	1.2452	0.0000		3.3978	1.2539	0.0000
H	3.3781	-1.2452	0.0000		3.3978	-1.2539	0.0000
H	1.2424	-2.4903	0.0000		1.2496	-2.5038	0.0000

2.10. Anthracene

	S_0			S_1		
X	Y	Z		X	Y	Z
C	-2.4795	-1.4073	0.0000	-2.4797	-1.3997	0.0000
C	-1.2238	-0.7229	0.0000	-1.2441	-0.7223	0.0000
C	-0.0000	-1.4040	0.0000	-0.0000	-1.3977	0.0000
C	-1.2238	0.7229	0.0000	-1.2441	0.7223	0.0000
C	0.0000	1.4040	0.0000	0.0000	1.3977	0.0000
C	1.2238	0.7229	0.0000	1.2441	0.7223	0.0000
C	1.2238	-0.7229	0.0000	1.2441	-0.7223	0.0000
C	-3.6605	-0.7132	0.0000	-3.7018	-0.6952	0.0000
C	-2.4795	1.4073	0.0000	-2.4797	1.3997	0.0000
H	-0.0000	2.4921	0.0000	-0.0000	2.4860	0.0000
C	2.4795	1.4073	0.0000	2.4797	1.3997	0.0000
C	2.4795	-1.4073	0.0000	2.4797	-1.3997	0.0000
C	3.6605	-0.7132	0.0000	3.7018	-0.6952	0.0000
C	3.6605	0.7132	0.0000	3.7018	0.6952	0.0000
H	2.4774	2.4946	0.0000	2.4829	2.4867	0.0000
H	2.4774	-2.4946	0.0000	2.4829	-2.4867	0.0000
H	4.6071	-1.2464	0.0000	4.6383	-1.2445	0.0000
H	4.6071	1.2464	0.0000	4.6383	1.2445	0.0000
C	-3.6605	0.7132	0.0000	-3.7018	0.6952	0.0000
H	-2.4774	-2.4946	0.0000	-2.4829	-2.4867	0.0000
H	0.0000	-2.4921	0.0000	0.0000	-2.4860	0.0000
H	-4.6071	-1.2464	0.0000	-4.6383	-1.2445	0.0000
H	-2.4774	2.4946	0.0000	-2.4829	2.4867	0.0000
H	-4.6071	1.2464	0.0000	-4.6383	1.2445	0.0000

2.11. Tetracene

	S_0			S_1		
X	Y	Z		X	Y	Z
C	-1.2354	-1.4068	0.0000	-1.2337	-1.4011	0.0000
C	-0.0000	-0.7265	0.0000	-0.0000	-0.7266	0.0000
C	1.2354	-1.4068	0.0000	1.2337	-1.4011	0.0000
C	0.0000	0.7265	0.0000	0.0000	0.7266	0.0000
C	1.2354	1.4068	0.0000	1.2337	1.4011	0.0000
C	2.4505	0.7262	0.0000	2.4771	0.7225	0.0000
C	2.4505	-0.7262	0.0000	2.4771	-0.7225	0.0000

C	-2.4505	-0.7262	0.0000	-2.4771	-0.7225	0.0000
C	-1.2354	1.4068	0.0000	-1.2337	1.4011	0.0000
H	1.2354	2.4948	0.0000	1.2349	2.4891	0.0000
C	3.7113	1.4096	0.0000	3.7144	1.4011	0.0000
C	3.7113	-1.4096	0.0000	3.7144	-1.4011	0.0000
C	4.8889	-0.7155	0.0000	4.9232	-0.7003	0.0000
C	4.8889	0.7155	0.0000	4.9232	0.7003	0.0000
H	3.7095	2.4969	0.0000	3.7161	2.4882	0.0000
H	3.7095	-2.4969	0.0000	3.7161	-2.4882	0.0000
H	5.8363	-1.2470	0.0000	5.8629	-1.2445	0.0000
H	5.8363	1.2470	0.0000	5.8629	1.2445	0.0000
C	-2.4505	0.7262	0.0000	-2.4771	0.7225	0.0000
H	-1.2354	-2.4948	0.0000	-1.2350	-2.4891	0.0000
H	1.2354	-2.4948	0.0000	1.2350	-2.4891	0.0000
C	-3.7113	-1.4096	0.0000	-3.7144	-1.4011	0.0000
H	-1.2354	2.4948	0.0000	-1.2349	2.4891	0.0000
C	-3.7113	1.4096	0.0000	-3.7144	1.4011	0.0000
C	-4.8889	-0.7155	0.0000	-4.9232	-0.7003	0.0000
C	-4.8889	0.7155	0.0000	-4.9232	0.7003	0.0000
H	-3.7095	-2.4969	0.0000	-3.7161	-2.4882	0.0000
H	-3.7095	2.4969	0.0000	-3.7161	2.4882	0.0000
H	-5.8363	-1.2470	0.0000	-5.8629	-1.2445	0.0000
H	-5.8363	1.2470	0.0000	-5.8629	1.2445	0.0000

2.12. Pentacene

	S_0			S_1		
	X	Y	Z	X	Y	Z
C	3.6784	0.7279	0.0008	3.7070	0.7212	0.0007
C	3.6779	-0.7284	0.0025	3.7075	-0.7206	0.0029
C	4.9414	1.4112	-0.0054	4.9462	1.4031	-0.0002
C	2.4676	1.4082	0.0043	2.4652	1.4058	-0.0037
C	4.9415	-1.4118	0.0025	4.9462	-1.4036	-0.0036
C	2.4669	-1.4092	-0.0075	2.4664	-1.4050	0.0006
C	6.1155	-0.7152	-0.0023	6.1485	-0.7043	-0.0013
C	6.1171	0.7172	-0.0015	6.1482	0.7029	-0.0001
C	1.2262	0.7278	0.0023	1.2375	0.7271	0.0030
C	1.2264	-0.7298	0.0009	1.2384	-0.7252	0.0007
C	0.0004	1.4100	-0.0029	-0.0004	1.4063	0.0032
C	-0.0004	-1.4087	0.0100	0.0003	-1.4064	-0.0010
C	-1.2258	0.7291	0.0007	-1.2379	0.7253	-0.0005
C	-1.2267	-0.7284	0.0009	-1.2381	-0.7271	0.0010
C	-2.4675	1.4089	0.0080	-2.4654	1.4051	0.0007
C	-2.4674	-1.4088	-0.0046	-2.4665	-1.4055	0.0036
C	-3.6783	0.7280	0.0014	-3.7079	0.7199	-0.0014
C	-3.6781	-0.7274	-0.0003	-3.7069	-0.7214	-0.0013
C	-4.9423	1.4106	-0.0044	-4.9468	1.4059	0.0025
C	-4.9404	-1.4131	0.0051	-4.9453	-1.4013	0.0006
C	-6.1144	0.7153	-0.0038	-6.1473	0.7021	-0.0004
C	-6.1181	-0.7169	-0.0014	-6.1496	-0.7053	-0.0034
H	4.9435	2.4992	0.0001	4.9473	2.4886	-0.0006
H	2.4691	2.4960	-0.0001	2.4693	2.4906	0.0017
H	4.9442	-2.4977	-0.0016	4.9466	-2.4902	0.0004

H	2.4676	-2.4972	0.0028	2.4702	-2.4892	0.0007
H	7.0633	-1.2481	-0.0024	7.0882	-1.2466	-0.0010
H	7.0632	1.2484	-0.0017	7.0872	1.2471	-0.0023
H	0.0017	2.4957	0.0035	-0.0019	2.4906	0.0005
H	-0.0014	-2.4980	-0.0008	0.0017	-2.4885	0.0019
H	-2.4691	2.4978	0.0002	-2.4685	2.4894	0.0010
H	-2.4668	-2.4953	0.0027	-2.4707	-2.4908	-0.0002
H	-4.9431	2.4977	-0.0001	-4.9452	2.4884	-0.0011
H	-4.9389	-2.4990	-0.0020	-4.9482	-2.4905	-0.0008
H	-7.0657	1.2449	-0.0024	-7.0880	1.2482	-0.0018
H	-7.0676	-1.2408	-0.0034	-7.0874	-1.2458	-0.0009

2.13. Hexacene

	S_0			S_1		
	X	Y	Z	X	Y	Z
C	-0.0001	-0.7322	0.002	-0.0006	-0.7311	-0.0017
C	-0.0001	0.7308	0.002	0.0007	0.7280	-0.0006
C	1.2320	1.4088	-0.004	1.2309	1.4099	0.0024
C	2.4545	0.7309	0.004	2.4713	0.7263	-0.0009
C	2.4539	-0.7307	0.005	2.4729	-0.7294	-0.0012
C	1.2323	-1.4090	-0.003	1.2307	-1.4016	0.0034
C	-1.2324	-1.4093	-0.002	-1.2297	-1.4048	0.0006
C	-1.2325	1.4085	-0.003	-1.2319	1.4072	-0.0002
H	1.2319	2.4978	0.001	1.2318	2.4904	-0.0006
C	3.6987	1.4089	-0.003	3.6984	1.4065	0.0007
C	3.6980	-1.4069	-0.002	3.6950	-1.4040	0.0012
H	1.2329	-2.4986	0.002	1.2313	-2.4940	-0.0002
C	-2.4544	0.7306	0.003	-2.4720	0.7283	0.0011
C	-2.4543	-0.7310	0.000	-2.4723	-0.7273	-0.0006
H	-1.2334	-2.4987	-0.000	-1.2312	-2.4926	-0.0004
H	-1.2331	2.4975	0.001	-1.2321	2.4915	0.0002
C	-3.6986	1.4081	-0.004	-3.6970	1.4030	0.0004
C	-3.6981	-1.4079	-0.007	-3.6964	-1.4074	-0.0010
C	4.9073	0.7294	0.000	4.9352	0.7224	-0.0011
C	4.9072	-0.7296	0.001	4.9365	-0.7227	0.0006
H	3.6992	2.4977	0.000	3.6998	2.4909	-0.0008
H	3.7000	-2.4966	0.003	3.6991	-2.4921	0.0009
C	6.1728	1.4104	-0.000	6.1771	1.4021	0.0006
C	6.1723	-1.4093	0.002	6.1786	-1.4052	0.0015
C	7.3471	-0.7175	-0.001	7.3728	-0.7074	-0.0007
C	7.3475	0.7171	-0.001	7.3753	0.7093	-0.0012
H	6.1718	2.4979	-0.002	6.1780	2.4921	-0.0015
H	6.1702	-2.4973	0.001	6.1786	-2.4907	0.0007
H	8.2951	-1.2480	0.000	8.3165	-1.2442	0.0004
H	8.2966	1.2464	-0.002	8.3143	1.2439	-0.0008
C	-4.9068	-0.7292	0.005	-4.9359	-0.7221	0.0005
C	-4.9075	0.7298	0.000	-4.9359	0.7232	-0.0010
H	-3.6994	2.4977	0.001	-3.6995	2.4924	0.0005
H	-3.7002	-2.4968	-0.001	-3.6994	-2.4906	-0.0008
C	-6.1719	-1.4092	-0.005	-6.1786	-1.4048	-0.0005
C	-6.1730	1.4104	-0.001	-6.1770	1.4023	0.0002

C	-7.3475	0.7168	0.001	-7.3747	0.7092	0.0017
C	-7.3467	-0.7178	0.001	-7.3736	-0.7078	-0.0016
H	-6.1701	-2.4972	-0.001	-6.1785	-2.4910	-0.0011
H	-6.1707	2.4981	0.002	-6.1780	2.4920	0.0010
H	-8.2957	1.2475	0.002	-8.3151	1.2440	0.0002
H	-8.2949	-1.2481	0.000	-8.3156	-1.2439	-0.0002