On the performance of the Kohn-Sham orbital approach in the calculation of

electron transfer parameters. Three state model

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Fig. S1 π-stacked and T-shape structures considered in the paper.

π1	π2	π3
π4	π5	π6
T1	T2	T3
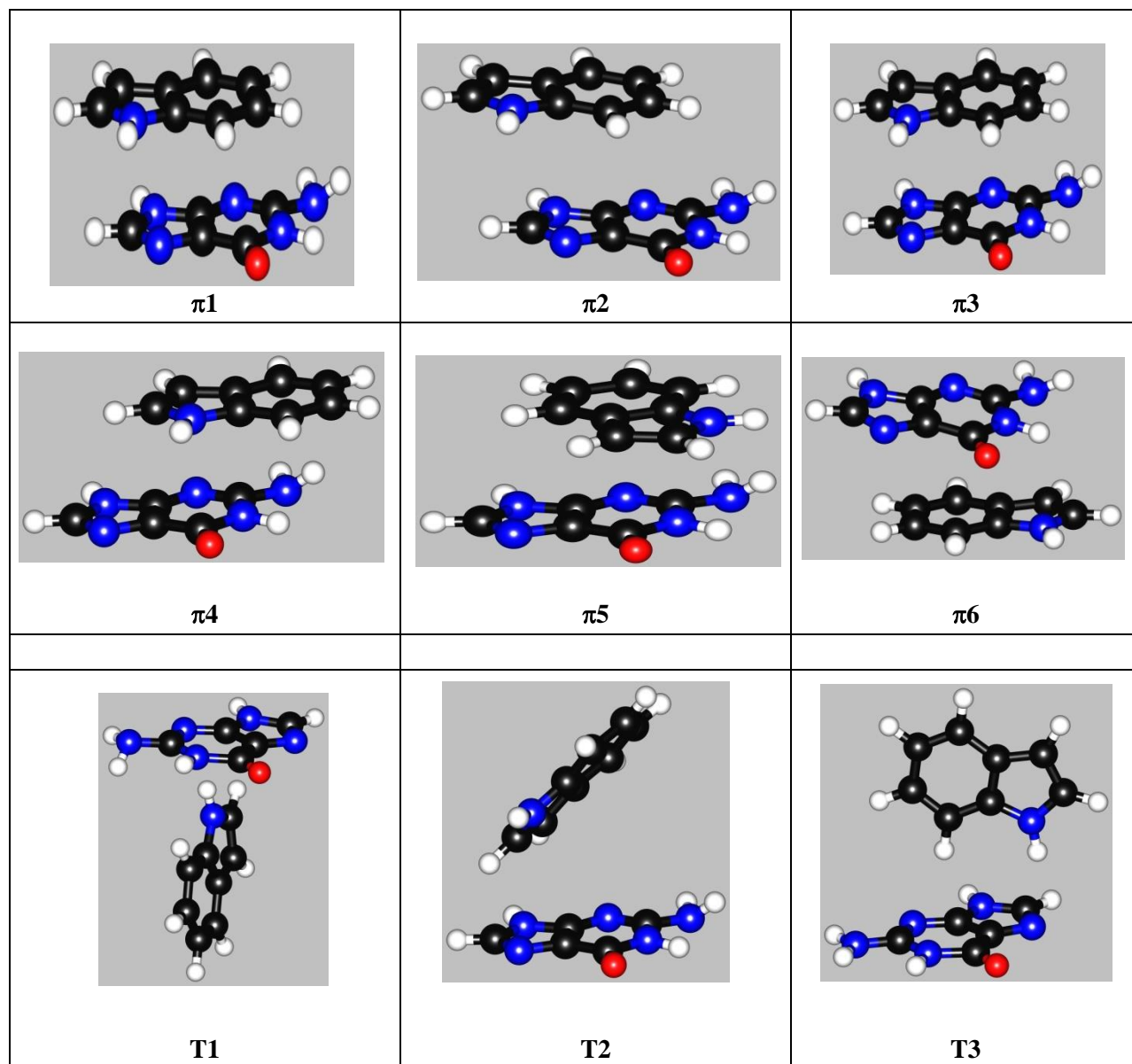
Table S2 RMS deviation in eV (RMSD) between the orbital-based couplings and the MS-CASPT2 values and linear regression analysis for the 10 DFT functionals and HF data

Method	Coupling	RMSD	R^2	slope	y-intercept
CAM-B3LYP	V_{GS-CT}	0.0217	0.9549	1.1648	-0.0146
	V_{ES-CT}	0.0288	0.9304	0.8603	-0.0034
wB97XD	V_{GS-CT}	0.0217	0.9553	1.1657	-0.0148
	V_{ES-CT}	0.0289	0.9292	0.8552	-0.0027
M062X	V_{GS-CT}	0.0277	0.9546	1.1865	-0.0148
	V_{ES-CT}	0.0233	0.9294	0.8976	-0.0051
LC-BLYP	V_{GS-CT}	0.0208	0.9582	1.2879	-0.0132
	V_{ES-CT}	0.0336	0.9537	0.9844	-0.0054
LC-wPBE	V_{GS-CT}	0.0286	0.9497	1.2417	-0.0161
	V_{ES-CT}	0.0259	0.9337	0.9084	-0.0036
PBE0	V_{GS-CT}	0.0194	0.9513	1.0716	-0.0155
	V_{ES-CT}	0.0361	0.9114	0.7806	-0.0029
B3LYP	V_{GS-CT}	0.0205	0.9484	1.0479	-0.0157
	V_{ES-CT}	0.0383	0.9054	0.7543	-0.0022
M06L	V_{GS-CT}	0.0269	0.9422	0.9591	-0.0163
	V_{ES-CT}	0.0437	0.9016	0.6953	-0.0023
HF	V_{GS-CT}	0.0479	0.9492	1.2441	0.0127
	V_{ES-CT}	0.0306	0.9756	1.1894	0.0035
BP86	V_{GS-CT}	0.0298	0.9228	0.9711	-0.0189
	V_{ES-CT}	0.0489	0.8420	0.6353	0.0031
BLYP	V_{GS-CT}	0.0303	0.9235	0.9592	-0.0184
	V_{ES-CT}	0.0496	0.8451	0.6275	0.0028

Table S3 – Calculated ET parameters (diabatic free energies and couplings) for the $\pi 1$ conformer different methods. (eV)

Method	Ect-Egs	Ees-Ect	Ees-Egs	Vgs-ct	Vct-es
CASPT2	0.1690	0.3311	0.5000	0.0666	0.3006
HF	0.2560	0.2830	0.5390	0.1307	0.3603
BP86	0.0460	0.4340	0.4800	0.0026	0.2226
BLYP	0.0670	0.4080	0.4750	0.0032	0.2191
B3LYP	0.0930	0.3920	0.4850	0.0182	0.2491
PBE0	0.0660	0.4270	0.4930	0.0208	0.2564
M06L	0.0560	0.4130	0.4690	0.0114	0.2312
M062X	0.1060	0.4120	0.5180	0.0275	0.2899
LC-BLYP	0.1440	0.3720	0.5160	0.0387	0.3115
CAM-B3LYP	0.1020	0.4040	0.5060	0.0281	0.2784
wB97XD	0.0830	0.4300	0.5130	0.0282	0.2776
LC-wPBE	0.0700	0.4490	0.5190	0.0279	0.2935

Table S4 – Calculated ET parameters (diabatic free energies and couplings) for the $\pi 2$ conformer different methods. (eV)

Method	Ect-Egs	Ees-Ect	Ees-Egs	Vgs-ct	Vct-es
CASPT2	0.3447	0.0559	0.4006	0.2280	0.1466
HF	0.4860	0.0300	0.5160	0.2846	0.1924
BP86	0.2320	0.2190	0.4510	0.2108	0.0506
BLYP	0.2540	0.1920	0.4460	0.2085	0.0503
B3LYP	0.2900	0.1650	0.4550	0.2296	0.0703
PBE0	0.2640	0.2000	0.4640	0.2347	0.0738
M06L	0.2470	0.1960	0.4430	0.2052	0.0645
M062X	0.3010	0.1850	0.4860	0.2605	0.0890
LC-BLYP	0.3510	0.1290	0.4800	0.2824	0.1039
CAM-B3LYP	0.3040	0.1700	0.4740	0.2564	0.0854
wB97XD	0.2820	0.1990	0.4810	0.2576	0.0848
LC-wPBE	0.2710	0.2130	0.4840	0.2697	0.0898

Table S5 – Calculated ET parameters (diabatic free energies and couplings) for the π3 conformer different methods. (eV)

Method	Ect-Egs	Ees-Ect	Ees-Egs	Vgs-ct	Vct-es
CASPT2	0.0162	0.2799	0.2961	0.1104	0.1178
HF	0.1480	0.2830	0.4310	0.1680	0.1404
BP86	-0.0450	0.4670	0.4220	0.1216	0.0697
BLYP	-0.0260	0.4420	0.4160	0.1199	0.0698
B3LYP	0.0000	0.4170	0.4170	0.1320	0.0798
PBE0	-0.0260	0.4500	0.4240	0.1355	0.0812
M06L	-0.0380	0.4420	0.4040	0.1207	0.0651
M062X	0.0080	0.4330	0.4410	0.1529	0.0919
LC-BLYP	0.0480	0.3850	0.4330	0.1712	0.1085
CAM-B3LYP	0.0080	0.4240	0.4320	0.1502	0.0940
wB97XD	-0.0120	0.4510	0.4390	0.1499	0.0945
LC-wPBE	-0.0220	0.4640	0.4420	0.1639	0.0992

Table S6 – Calculated ET parameters (diabatic free energies and couplings) for the $\pi 4$ conformer different methods. (eV)

Method	Ect-Egs	Ees-Ect	Ees-Egs	Vgs-ct	Vct-es
CASPT2	0.1908	0.2647	0.4555	0.1407	0.0043
HF	0.3080	0.2620	0.5700	0.2056	0.0016
BP86	0.0490	0.4340	0.4830	0.1077	0.0352
BLYP	0.0690	0.4070	0.4760	0.1059	0.0344
B3LYP	0.1080	0.3850	0.4930	0.1246	0.0331
PBE0	0.0850	0.4200	0.5050	0.1292	0.0332
M06L	0.0560	0.4180	0.4740	0.1147	0.0285
M062X	0.1170	0.4110	0.5280	0.1470	0.0344
LC-BLYP	0.1570	0.3640	0.5210	0.1619	0.0314
CAM-B3LYP	0.1170	0.3970	0.5140	0.1420	0.0333
wB97XD	0.0960	0.4290	0.5250	0.1424	0.0339
LC-wPBE	0.0840	0.4440	0.5280	0.1516	0.0327

Table S7 – Calculated ET parameters (diabatic free energies and couplings) for the π5 conformer different methods. (eV)

Method	Ect-Egs	Ees-Ect	Ees-Egs	Vgs-ct	Vct-es
CASPT2	0.1463	0.2297	0.3760	0.2124	0.0079
HF	0.3560	0.2720	0.6280	0.2787	0.0544
BP86	0.1020	0.4100	0.5120	0.1835	0.0388
BLYP	0.1280	0.3810	0.5090	0.1816	0.0382
B3LYP	0.1610	0.3660	0.5270	0.2033	0.0270
PBE0	0.1320	0.4030	0.5350	0.2083	0.0255
M06L	0.1150	0.3960	0.5110	0.1863	0.0238
M062X	0.1690	0.3890	0.5580	0.2333	0.0234
LC-BLYP	0.2060	0.3500	0.5560	0.2588	0.0172
CAM-B3LYP	0.1690	0.3800	0.5490	0.2295	0.0236
wB97XD	0.1460	0.4090	0.5550	0.2281	0.0246
LC-wPBE	0.1260	0.4290	0.5550	0.2458	0.0247

Table S8 – Calculated ET parameters (diabatic free energies and couplings) for the π6 conformer different methods. (eV)

Method	Ect-Egs	Ees-Ect	Ees-Egs	Vgs-ct	Vct-es
CASPT2	-0.0123	0.2439	0.2317	0.0192	0.0448
HF	0.1740	0.1300	0.3040	0.0421	0.0443
BP86	-0.0590	0.4350	0.3760	0.0038	0.0407
BLYP	-0.0360	0.4090	0.3730	0.0034	0.0384
B3LYP	-0.0070	0.3710	0.3640	0.0090	0.0354
PBE0	-0.0380	0.4060	0.3680	0.0100	0.0362
M06L	-0.0490	0.4010	0.3520	0.0086	0.0401
M062X	-0.0040	0.3840	0.3800	0.0150	0.0352
LC-BLYP	0.0380	0.3260	0.3640	0.0191	0.0379
CAM-B3LYP	-0.0010	0.3710	0.3700	0.0138	0.0359
wB97XD	-0.0250	0.4030	0.3780	0.0139	0.0363
LC-wPBE	-0.0400	0.4200	0.3800	0.0149	0.0388

Table S9 – Calculated ET parameters (diabatic free energies and couplings) for the T1 conformer different methods. (eV)

Method	Ect-Egs	Ees-Ect	Ees-Egs	Vgs-ct	Vct-es
CASPT2	0.7216	-0.3266	0.3950	0.0757	0.0520
HF	0.8780	-0.4000	0.4780	0.0732	0.0472
BP86	0.6500	-0.2000	0.4500	0.0610	0.0177
BLYP	0.6560	-0.2120	0.4440	0.0611	0.0170
B3LYP	0.6960	-0.2490	0.4470	0.0656	0.0220
PBE0	0.6920	-0.2360	0.4560	0.0662	0.0233
M06L	0.6300	-0.1970	0.4330	0.0562	0.0227
M062X	0.7200	-0.2480	0.4720	0.0730	0.0285
LC-BLYP	0.7500	-0.2890	0.4610	0.0797	0.0353
CAM-B3LYP	0.7060	-0.2450	0.4610	0.0730	0.0282
wB97XD	0.6850	-0.2150	0.4700	0.0729	0.0294
LC-wPBE	0.6860	-0.2160	0.4700	0.0755	0.0329

Table S10 – Calculated ET parameters (diabatic free energies and couplings) for the T2 conformer different methods. (eV)

Method	Ect-Egs	Ees-Ect	Ees-Egs	Vgs-ct	Vct-es
CASPT2	0.5105	-0.0114	0.4991	0.1259	0.0315
HF	0.6080	-0.0590	0.5490	0.1561	0.0366
BP86	0.3260	0.1400	0.4660	0.0932	0.0053
BLYP	0.3400	0.1210	0.4610	0.0922	0.0049
B3LYP	0.3850	0.0880	0.4730	0.1057	0.0003
PBE0	0.3720	0.1100	0.4820	0.1089	0.0001
M06L	0.3110	0.1410	0.4520	0.0950	0.0003
M062X	0.4020	0.1000	0.5020	0.1240	0.0012
LC-BLYP	0.4440	0.0570	0.5010	0.1362	0.0057
CAM-B3LYP	0.3970	0.0960	0.4930	0.1204	0.0026
wB97XD	0.3720	0.1290	0.5010	0.1205	0.0031
LC-wPBE	0.3680	0.1380	0.5060	0.1283	0.0023

Table S11 – Calculated ET parameters (diabatic free energies and couplings) for the T3 conformer different methods. (eV)

Method	Ect-Egs	Ees-Ect	Ees-Egs	Vgs-ct	Vct-es
CASPT2	0.7441	-0.3167	0.4274	0.0197	0.0195
HF	0.8980	-0.3970	0.5010	0.0180	0.0164
BP86	0.6010	-0.1350	0.4660	0.0159	0.0081
BLYP	0.6080	-0.1480	0.4600	0.0160	0.0083
B3LYP	0.6590	-0.1940	0.4650	0.0170	0.0097
PBE0	0.6550	-0.1820	0.4730	0.0170	0.0097
M06L	0.5800	-0.1310	0.4490	0.0131	0.0074
M062X	0.6880	-0.1970	0.4910	0.0183	0.0110
LC-BLYP	0.7310	-0.2490	0.4820	0.0193	0.0132
CAM-B3LYP	0.6770	-0.1970	0.4800	0.0183	0.0115
wB97XD	0.6540	-0.1650	0.4890	0.0178	0.0113
LC-wPBE	0.6560	-0.1660	0.4900	0.0178	0.0117

Cartesian coordinates (in Å) for π- stacked and T-shape guanine-indole pairs.

Complex π1

7	0.266800000	-2.636000000	-0.004000000
6	1.634300000	-2.773600000	0.002000000
1	2.112000000	-3.744900000	-0.001000000
7	2.269100000	-1.611800000	0.016000000
6	1.253000000	-0.681900000	0.018000000
6	1.326800000	0.758300000	0.009000000
8	2.290900000	1.513900000	-0.003000000
7	0.000000000	1.291900000	0.000000000
1	-0.028600000	2.304100000	-0.098000000
6	-1.175600000	0.583300000	0.006000000
7	-2.337700000	1.335400000	-0.074000000
1	-2.354500000	2.168000000	0.506000000
1	-3.155800000	0.753000000	0.073000000
7	-1.242900000	-0.725600000	0.015000000
6	0.000000000	-1.291900000	0.000000000
1	-0.429900000	-3.371900000	-0.018000000
6	0.365400000	-2.784100000	3.380000000
6	1.739800000	-2.838300000	3.380000000
6	0.000000000	-1.401500000	3.380000000
1	2.405500000	-3.692000000	3.380000000
7	2.246500000	-1.555100000	3.380000000
6	1.208600000	-0.650200000	3.380000000
6	-1.226100000	-0.708800000	3.380000000
1	3.229300000	-1.317400000	3.383000000
6	1.226800000	0.750700000	3.380000000
6	-1.213700000	0.678700000	3.380000000
1	-2.167700000	-1.254700000	3.380000000
1	2.160900000	1.309100000	3.380000000
6	0.000000000	1.401500000	3.380000000
1	-2.154200000	1.224500000	3.380000000
1	-0.027000000	2.488600000	3.380000000
1	-0.301100000	-3.637000000	3.380000000

Complex π2

7	0.266800000	-2.636000000	-0.004000000
6	1.634300000	-2.773600000	0.002000000
1	2.112000000	-3.744900000	-0.001000000
7	2.269100000	-1.611800000	0.016000000
6	1.253000000	-0.681900000	0.018000000
6	1.326800000	0.758300000	0.009000000
8	2.290900000	1.513900000	-0.003000000
7	0.000000000	1.291900000	0.000000000
1	-0.028600000	2.304100000	-0.098000000
6	-1.175600000	0.583300000	0.006000000
7	-2.337700000	1.335400000	-0.074000000
1	-2.354500000	2.168000000	0.506000000
1	-3.155800000	0.753000000	0.073000000
7	-1.242900000	-0.725600000	0.015000000
6	0.000000000	-1.291900000	0.000000000
1	-0.429900000	-3.371900000	-0.018000000
6	2.365400000	-2.784100000	3.380000000
6	3.739800000	-2.838300000	3.380000000
6	2.000000000	-1.401500000	3.380000000
1	4.405500000	-3.692000000	3.380000000
7	4.246500000	-1.555100000	3.380000000
6	3.208600000	-0.650200000	3.380000000
6	0.773900000	-0.708800000	3.380000000
1	5.229300000	-1.317400000	3.383000000
6	3.226800000	0.750700000	3.380000000
6	0.786300000	0.678700000	3.380000000
1	-0.167700000	-1.254700000	3.380000000
1	4.160900000	1.309100000	3.380000000
6	2.000000000	1.401500000	3.380000000
1	-0.154200000	1.224500000	3.380000000
1	1.973000000	2.488600000	3.380000000
1	1.698900000	-3.637000000	3.380000000

Complex π3

7	0.266800000	-2.636000000	-0.004000000
6	1.634300000	-2.773600000	0.002000000
1	2.112000000	-3.744900000	-0.001000000
7	2.269100000	-1.611800000	0.016000000
6	1.253000000	-0.681900000	0.018000000
6	1.326800000	0.758300000	0.009000000
8	2.290900000	1.513900000	-0.003000000
7	0.000000000	1.291900000	0.000000000
1	-0.028600000	2.304100000	-0.098000000
6	-1.175600000	0.583300000	0.006000000
7	-2.337700000	1.335400000	-0.074000000
1	-2.354500000	2.168000000	0.506000000
1	-3.155800000	0.753000000	0.073000000
7	-1.242900000	-0.725600000	0.015000000
6	0.000000000	-1.291900000	0.000000000
1	-0.429900000	-3.371900000	-0.018000000
6	0.365400000	-4.484100000	3.380000000
6	1.739800000	-4.538300000	3.380000000
6	0.000000000	-3.101500000	3.380000000
1	2.405500000	-5.392000000	3.380000000
7	2.246500000	-3.255100000	3.380000000
6	1.208600000	-2.350200000	3.380000000
6	-1.226100000	-2.408800000	3.380000000
1	3.229300000	-3.017400000	3.383000000
6	1.226800000	-0.949300000	3.380000000
6	-1.213700000	-1.021300000	3.380000000
1	-2.167700000	-2.954700000	3.380000000
1	2.160900000	-0.390900000	3.380000000
6	0.000000000	-0.298500000	3.380000000
1	-2.154200000	-0.475500000	3.380000000
1	-0.027000000	0.788600000	3.380000000
1	-0.301100000	-5.337000000	3.380000000

Complex π4

7	0.266800000	-2.636000000	-0.004000000
6	1.634300000	-2.773600000	0.002000000
1	2.112000000	-3.744900000	-0.001000000
7	2.269100000	-1.611800000	0.016000000
6	1.253000000	-0.681900000	0.018000000
6	1.326800000	0.758300000	0.009000000
8	2.290900000	1.513900000	-0.003000000
7	0.000000000	1.291900000	0.000000000
1	-0.028600000	2.304100000	-0.098000000
6	-1.175600000	0.583300000	0.006000000
7	-2.337700000	1.335400000	-0.074000000
1	-2.354500000	2.168000000	0.506000000
1	-3.155800000	0.753000000	0.073000000
7	-1.242900000	-0.725600000	0.015000000
6	0.000000000	-1.291900000	0.000000000
1	-0.429900000	-3.371900000	-0.018000000
6	0.365400000	-0.084100000	3.380000000
6	1.739800000	-0.138300000	3.380000000
6	0.000000000	1.298500000	3.380000000
1	2.405500000	-0.992000000	3.380000000
7	2.246500000	1.144900000	3.380000000
6	1.208600000	2.049800000	3.380000000
6	-1.226100000	1.991200000	3.380000000
1	3.229300000	1.382600000	3.383000000
6	1.226800000	3.450700000	3.380000000
6	-1.213700000	3.378700000	3.380000000
1	-2.167700000	1.445300000	3.380000000
1	2.160900000	4.009100000	3.380000000
6	0.000000000	4.101500000	3.380000000
1	-2.154200000	3.924500000	3.380000000
1	-0.027000000	5.188600000	3.380000000
1	-0.301100000	-0.937000000	3.380000000

Complex π5

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7       0.266800000      -2.636000000      -0.004000000
6       1.634300000      -2.773600000       0.002000000
1       2.112000000      -3.744900000      -0.001000000
7       2.269100000      -1.611800000       0.016000000
6       1.253000000      -0.681900000       0.018000000
6       1.326800000       0.758300000       0.009000000
8       2.290900000       1.513900000      -0.003000000
7       0.000000000       1.291900000       0.000000000
1      -0.028600000       2.304100000      -0.098000000
6      -1.175600000       0.583300000       0.006000000
7      -2.337700000       1.335400000      -0.074000000
1      -2.354500000       2.168000000       0.506000000
1      -3.155800000       0.753000000       0.073000000
7      -1.242900000      -0.725600000       0.015000000
6       0.000000000      -1.291900000       0.000000000
1      -0.429900000      -3.371900000      -0.018000000
6       2.491200000       1.295600000       3.380000000
6       2.072100000       2.605600000       3.380000000
6       1.317000000       0.479300000       3.380000000
1       2.646600000       3.523200000       3.380000000
7       0.693000000       2.642900000       3.380000000
6       0.197600000       1.358100000       3.380000000
6       1.085400000      -0.909700000       3.380000000
1       0.133500000       3.485100000       3.383000000
6      -1.125000000       0.896100000       3.380000000
6      -0.222700000      -1.372600000       3.380000000
1       1.920400000      -1.607800000       3.380000000
1      -1.969200000       1.582800000       3.380000000
6      -1.317000000      -0.479300000       3.380000000
1      -0.413900000      -2.443100000       3.380000000
1      -2.329300000      -0.876500000       3.380000000
1       3.520600000       0.961000000       3.380000000
```

Complex π6

```
7         0.266800000    -2.636000000    -0.004000000
6         1.634300000    -2.773600000     0.002000000
1         2.112000000    -3.744900000    -0.001000000
7         2.269100000    -1.611800000     0.016000000
6         1.253000000    -0.681900000     0.018000000
6         1.326800000     0.758300000     0.009000000
8         2.290900000     1.513900000    -0.003000000
7         0.000000000     1.291900000     0.000000000
1        -0.028600000     2.304100000    -0.098000000
6        -1.175600000     0.583300000     0.006000000
7        -2.337700000     1.335400000    -0.074000000
1        -2.354500000     2.168000000     0.506000000
1        -3.155800000     0.753000000     0.073000000
7        -1.242900000    -0.725600000     0.015000000
6         0.000000000    -1.291900000     0.000000000
1        -0.429900000    -3.371900000    -0.018000000
6        -1.865300000     2.262000000    -3.190900000
6        -1.014500000     3.312200000    -2.935400000
6        -1.058300000     1.087300000    -3.308800000
1        -1.227300000     4.362400000    -2.781400000
7         0.283200000     2.846400000    -2.888800000
6         0.293200000     1.487800000    -3.113300000
6        -1.330800000    -0.271200000    -3.560200000
1         1.100700000     3.416800000    -2.719200000
6         1.362900000     0.584300000    -3.161200000
6        -0.274900000    -1.170300000    -3.608700000
1        -2.353900000    -0.609100000    -3.714000000
1         2.390600000     0.908500000    -3.009300000
6         1.058300000    -0.747300000    -3.411200000
1        -0.473000000    -2.221800000    -3.802100000
1         1.861800000    -1.478800000    -3.455900000
1        -2.941800000     2.328200000    -3.282600000
```

Complex T1

7	0.266800000	-2.636000000	-0.004000000
6	1.634300000	-2.773600000	0.002000000
1	2.112000000	-3.744900000	-0.001000000
7	2.269100000	-1.611800000	0.016000000
6	1.253000000	-0.681900000	0.018000000
6	1.326800000	0.758300000	0.009000000
8	2.290900000	1.513900000	-0.003000000
7	0.000000000	1.291900000	0.000000000
1	-0.028600000	2.304100000	-0.098000000
6	-1.175600000	0.583300000	0.006000000
7	-2.337700000	1.335400000	-0.074000000
1	-2.354500000	2.168000000	0.506000000
1	-3.155800000	0.753000000	0.073000000
7	-1.242900000	-0.725600000	0.015000000
6	0.000000000	-1.291900000	0.000000000
1	-0.429900000	-3.371900000	-0.018000000
6	-0.063500000	-2.784100000	5.020100000
6	-0.302100000	-2.838300000	3.666600000
6	0.000000000	-1.401500000	5.380000000
1	-0.417700000	-3.692000000	3.011000000
7	-0.390100000	-1.555100000	3.167600000
6	-0.209900000	-0.650200000	4.189800000
6	0.212900000	-0.708800000	6.587500000
1	-0.557800000	-1.317400000	2.199200000
6	-0.213000000	0.750700000	4.171800000
6	0.210800000	0.678700000	6.575300000
1	0.376400000	-1.254700000	7.514800000
1	-0.375200000	1.309100000	3.251900000
6	0.000000000	1.401500000	5.380000000
1	0.374100000	1.224500000	7.501500000
1	0.004700000	2.488600000	5.406600000
1	0.052300000	-3.637000000	5.676500000

Complex T2

```
7        0.266800000     -2.636000000     -0.004000000
6        1.634300000     -2.773600000      0.002000000
1        2.112000000     -3.744900000     -0.001000000
7        2.269100000     -1.611800000      0.016000000
6        1.253000000     -0.681900000      0.018000000
6        1.326800000      0.758300000      0.009000000
8        2.290900000      1.513900000     -0.003000000
7        0.000000000      1.291900000      0.000000000
1       -0.028600000      2.304100000     -0.098000000
6       -1.175600000      0.583300000      0.006000000
7       -2.337700000      1.335400000     -0.074000000
1       -2.354500000      2.168000000      0.506000000
1       -3.155800000      0.753000000      0.073000000
7       -1.242900000     -0.725600000      0.015000000
6        0.000000000     -1.291900000      0.000000000
1       -0.429900000     -3.371900000     -0.018000000
6        0.365400000     -1.789600000      3.247300000
6        1.739800000     -1.824400000      3.205700000
6        0.000000000     -0.900900000      4.306400000
1        2.405500000     -2.373200000      2.551800000
7        2.246500000     -0.999600000      4.188700000
6        1.208600000     -0.417900000      4.881900000
6       -1.226100000     -0.455600000      4.837000000
1        3.229300000     -0.849100000      4.372700000
6        1.226800000      0.482500000      5.955100000
6       -1.213700000      0.436300000      5.899900000
1       -2.167700000     -0.806500000      4.418800000
1        2.160900000      0.841500000      6.382800000
6        0.000000000      0.900900000      6.453600000
1       -2.154200000      0.787100000      6.318000000
1       -0.027000000      1.599600000      7.286400000
1       -0.301100000     -2.337800000      2.593900000
```

Complex T3

7	-1.722530000	2.459270000	1.191890000
6	-0.878800000	2.459270000	2.278330000
7	0.399690000	2.459270000	1.937070000
6	0.371980000	2.459270000	0.558950000
6	1.462800000	2.459270000	-0.381050000
8	2.676320000	2.459270000	-0.210300000
7	0.935190000	2.459270000	-1.711400000
6	-0.390570000	2.459270000	-2.074980000
7	-0.663430000	2.459270000	-3.410970000
7	-1.384710000	2.459270000	-1.216110000
6	-0.933930000	2.459270000	0.071220000
1	-1.253680000	2.459270000	3.293650000
1	1.661260000	2.459270000	-2.423280000
1	0.052680000	2.459270000	-4.118530000
1	-1.632920000	2.459270000	-3.688360000
1	-2.735730000	2.459270000	1.194260000
1	1.709130000	-1.816390000	3.622040000
1	0.771290000	-0.136580000	2.004170000
1	-0.306550000	-5.087480000	0.144800000
1	-0.650410000	-0.103670000	-0.448390000
1	-1.450240000	-4.114260000	-1.828170000
1	-1.621180000	-1.663380000	-2.123060000
1	1.157680000	-4.289860000	2.670740000
6	0.892890000	-3.345040000	2.213940000
6	1.185040000	-2.099110000	2.717920000
6	0.182560000	-3.146040000	0.988570000
7	0.690270000	-1.134700000	1.864420000
6	0.070150000	-1.740990000	0.794640000
6	-0.375970000	-4.007880000	0.025040000
6	-0.573970000	-1.181300000	-0.316520000
6	-1.015060000	-3.458880000	-1.077450000
6	-1.113330000	-2.059780000	-1.246960000