Supporting Information for

Can Domain-Based Local Pair Natural Orbitals Approaches Accurately Predict Phosphorescence Energies?

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S1 DFT Geometry Optimizations

To select a DFT functional for geometry optimizations, we tested three different exchange-correlation functionals: one belonging to the GGA class (BLYP), one hybrid (B3LYP) and one belonging to Minnesota family (M06-2X). Geometry optimizations of both the ground state (S_0) and the first excited triplet state (T_1) for the compounds in Figure 1 were performed using the def2-TZVPP basis set. The RI approximation for both Coulomb (J) and Exchange (K) integrals (RIJK option of ORCA 4.2.1) was used. Grimme's atom-pairwise dispersion correction with Becke-Johnson damping was used to correct the BLYP and B3LYP energies. The corresponding zero damping variant was used in M06-2X calculations. The main criterion for selecting the functional was the minimization of the DLPNO-CCSD(T1)/TightPNO total energy of both the singlet and triplet state. The aug-cc-pVTZ basis set was used in the corresponding DLPNO-CCSD(T1) calculations. Tables S1, S2 and S3 collect the results obtained.

Compound	Optimization Method	E_{S_0}	E_{T_1}
1a	B3LYP	-231.8193	-231.6746
	BLYP	-231.8195	-231.6748
	M062X	-231.8191	-231.6745
2a	B3LYP	-271.0654	-270.9248
	BLYP	-271.0655	-270.9248
	M06-2X	-271.0652	-270.9235
3a	B3LYP	-330.9604	-330.8162
	BLYP	-330.9603	-330.8161
	M06-2X	-330.9602	-330.8154
4a	B3LYP	-384.2386	-384.1183
	BLYP	-384.2387	-384.1044
	M06-2X	-384.2379	-384.1105
5a	B3LYP	-310.3112	-310.1742
	BLYP	-310.3113	-310.1743
	M06-2X	-310.3110	-310.1726
6a	B3LYP	-628.3587	-628.1842
	BLYP	-628.3576	-628.2311
	M06-2X	-628.3585	-628.2297
7a	B3LYP	-588.4861	-588.3822
	BLYP	-588.4856	-588.3814
	M06-2X	-588.4842	-588.3763

Table S1: DLPNO-CCSD(T) absolute energies (in Eh) of states S_0 and T_1 of compounds of Group A (Figure 1), calculated at optimized geometries obtained by different DFT functionals.

Compound	Optimization Method	E_{S_0}	E_{T_1}
	B3LYP	-385.1813	-385.0770
1b	BLYP	-385.1815	-385.0772
	M062X	-385.1810	-385.0766
	B3LYP	-931.0973	-930.9868
2b	BLYP	-931.0969	-
	M062X	-931.0945	-930.9852
	B3LYP	-651.9876	-651.8874
3b	BLYP	-651.9839	-651.8868
	M062X	-651.9865	-651.8847
	B3LYP	-844.3228	-844.2183
4b	BLYP	-844.3229	-844.2182
	M062X	-844.3225	-844.2178
	B3LYP	-495.7221	-495.6292
5b	BLYP	-495.7221	-495.6289
	M062X	-495.7219	-495.6289

Table S2: DLPNO-CCSD(T) absolute energies (in Eh) of states S_0 and T_1 of compounds of Group B (Figure 1), calculated at optimized geometries obtained by different DFT functionals.

Compound	Optimization Method	E_{S_0}	E_{T_1}
	B3LYP	-555.7813	-555.6684
1c	BLYP	-555.7814	-555.6682
	M062X	-555.7810	-555.6681
	B3LYP	-538.5372	-538.4627
2c	BLYP	-538.5375	-538.4629
	M062X	-538.5369	-538.4622
	B3LYP	-462.4549	-462.3378
1d	BLYP	-462.4552	-462.3381
	M062X	-462.4545	-462.3374
	B3LYP	-870.9533	-870.8431
2d	BLYP	-870.9524	-870.8341
	M062X	-870.9506	-870.8407
	B3LYP	-898.2209	-898.1565
3d	BLYP	-898.2212	-898.1567
	M062X	-898.2203	-898.1557
	B3LYP	-401.2109	-401.1031
1e	BLYP	-401.2112	-401.1032
	M062X	-401.2105	-401.1009

Table S3: DLPNO-CCSD(T) absolute energies (in Eh) of states S_0 and T_1 of compounds of Groups C, D and E (Figure 1), calculated at optimized geometries obtained by different DFT functionals.

The energy difference between structures optimized with different functionals is quite small (of the order of 10^{-4} Eh). However, the BLYP and the B3LYP functionals provide geometries that are generally closer to the "true" DLPNO-CCSD(T) minimum with respect to M06-2X. As BLYP calculations were found to be harder to converge for some systems (e.g., we could not obtain the BLYP structure of the triplet state of compound **2b**, Figure 1), we selected B3LYP for geometry optimizations and for the corresponding zero-point energy corrections. The corresponding B3LYP optimized geometries, for each compound of Figure 1 and for each spin state, are reported in the following tables. All cartesian coordinates are in Å.

1a S_0

Atom	x	y	z
C	-1.204511	0.695434	-0.000039
C	-1.204528	-0.695427	-0.000009
C	-0.000009	-1.390859	0.000032
C	1.204512	-0.695433	0.000040
C	1.204528	0.695426	0.000008
C	0.000007	1.390860	-0.000031
H	-2.141625	1.236488	-0.000068
H	-2.141648	-1.236467	-0.000019
H	-0.000010	-2.472950	0.000058
H	2.141624	-1.236489	0.000072
H	2.141647	1.236468	0.000012
H	0.000011	2.472950	-0.000053

1a T_1

Atom	x	y	z
C	-1.244371	0.718446	-0.000038
C	-1.258653	-0.664183	-0.000025
C	0.054113	-1.422115	0.000048
C	1.244371	-0.718446	0.000039
C	1.258653	0.664183	-0.000006
C	-0.054113	1.422115	-0.000016
H	-2.182351	1.259999	-0.000069
H	-2.185851	-1.217167	-0.000074
H	0.038805	-2.501584	0.000115
H	2.182351	-1.259999	0.000070
H	2.185851	1.217167	-0.000032
H	-0.038805	2.501584	-0.000008

2a S_0

Atom	x	y	z
C	0.441529	0.547596	-0.145273
C	-1.270056	-1.602875	0.425255
C	0.953254	-0.704787	0.189261
C	-0.945708	0.704268	-0.189131
C	0.107440	-1.772589	0.472566
C	-1.794451	-0.357611	0.092582
C	1.352282	1.705976	-0.452593
H	-1.930112	-2.431342	0.645052
H	2.026316	-0.846235	0.228583
H	-1.363328	1.670164	-0.447191
H	0.526744	-2.736486	0.730092
H	-2.866478	-0.214511	0.052810
H	2.400010	1.418051	-0.374231
H	1.182590	2.083884	-1.463013
H	1.179965	2.536500	0.235228

2a T_1

Atom	x	y	z
C	0.515832	0.524569	-0.139129
C	-1.325326	-1.585463	0.420634
C	1.006316	-0.729663	0.195866
C	-0.991912	0.717285	-0.192814
C	0.168200	-1.788847	0.476973
C	-1.833627	-0.346856	0.089676
C	1.363290	1.696211	-0.449908
H	-1.978883	-2.416561	0.641250
H	2.079979	-0.874763	0.236139
H	-1.379183	1.691669	-0.453256
H	0.558709	-2.761007	0.736666
H	-2.906460	-0.203246	0.049796
H	2.425847	1.464797	-0.386593
H	1.149927	2.080998	-1.457129
H	1.147290	2.530880	0.231824

3a S_0

Atom	x	y	z
C	0.814855	1.027913	-0.272646
C	1.372251	-0.195618	0.054215
C	0.519175	-1.257226	0.335783
C	-0.860098	-1.084988	0.287787
C	-1.391553	0.156747	-0.043891
C	-0.552985	1.229089	-0.328344
F	1.636768	2.064756	-0.547647
H	2.447079	-0.303999	0.084734
H	0.937102	-2.221087	0.593241
H	-1.517707	-1.914545	0.507824
H	-2.463578	0.295484	-0.082495
H	-0.941309	2.203473	-0.588560

3a T_1

Atom	x	y	z
C	0.877088	1.003108	-0.265943
C	1.426375	-0.197860	0.054913
C	0.579761	-1.278120	0.341484
C	-0.915704	-1.065561	0.282514
C	-1.437580	0.157028	-0.044051
C	-0.603076	1.243958	-0.332349
F	1.638221	2.071300	-0.549501
H	2.502525	-0.301689	0.084199
H	0.973173	-2.247536	0.600390
H	-1.565331	-1.899917	0.503794
H	-2.510971	0.290255	-0.081216
H	-0.964479	2.225034	-0.594231

4a S_0

Atom	x	y	z
C	1.326970	1.177259	-0.311937
C	0.743631	2.526471	-0.672041
O	2.529649	1.015988	-0.267321
C	0.391533	0.048410	-0.012504
C	0.933787	-1.196387	0.320171
C	0.105538	-2.269688	0.605136
C	-1.277776	-2.113674	0.561496
C	-1.827458	-0.880564	0.231869
C	-0.996788	0.195679	-0.053844
H	1.557346	3.222308	-0.855445
H	0.118437	2.453460	-1.563868
H	0.114794	2.905522	0.135683
H	2.009584	-1.295609	0.348231
H	0.533745	-3.229470	0.861699
H	-1.924719	-2.951937	0.784078
H	-2.901542	-0.86908	0.197293
H	-1.436732	1.149140	-0.308695

4a T_1

Atom	x	y	z
C	1.219481	1.156831	-0.323527
C	0.766350	2.551645	-0.681438
O	2.526407	1.023029	-0.407260
C	0.381631	0.060818	-0.018987
C	0.933725	-1.208153	0.306391
C	0.111775	-2.274412	0.606925
C	-1.277764	-2.133452	0.597029
C	-1.834118	-0.894358	0.273728
C	-1.031458	0.186404	-0.034768
H	1.582990	3.262118	-0.564623
H	0.417706	2.596947	-1.717146
H	-0.045992	2.848399	-0.018010
H	2.008597	-1.327685	0.326029
H	0.553583	-3.230676	0.855969
H	-1.914991	-2.973570	0.835076
H	-2.909774	-0.774749	0.258912
H	-1.488151	1.130864	-0.294299

5a S_0

Atom	x	y	z
C	1.201225	2.307367	-0.613118
C	0.285152	1.152581	-0.306736
C	0.796560	-0.100497	0.027960
C	-0.031571	-1.184576	0.315628
C	-1.412286	-0.996108	0.263340
C	-1.940642	0.244844	-0.068145
C	-1.099365	1.312999	-0.351544
C	0.545972	-2.527804	0.674474
H	2.247853	2.015557	-0.533766
H	1.033929	2.685969	-1.623686
H	1.031371	3.138567	0.074510
H	1.871387	-0.236105	0.065703
H	-2.075227	-1.824113	0.483013
H	-3.013896	0.380251	-0.105829
H	-1.519377	2.277634	-0.609237
H	1.635175	-2.505434	0.670300
H	0.220479	-2.844315	1.667677
H	0.223258	-3.296818	-0.030544

5a T_1

Atom	x	y	z
C	1.206099	2.317119	-0.615642
C	0.366060	1.137510	-0.302640
C	0.866751	-0.109344	0.030431
C	0.050576	-1.190094	0.317293
C	-1.449688	-0.988266	0.261351
C	-1.970057	0.248540	-0.069176
C	-1.137540	1.314700	-0.352205
C	0.548081	-2.538430	0.677263
H	2.269746	2.089420	-0.553246
H	0.993951	2.700713	-1.623346
H	0.991238	3.151134	0.066909
H	1.942845	-0.245137	0.068229
H	-2.093556	-1.827328	0.484104
H	-3.044126	0.384062	-0.106928
H	-1.536156	2.285269	-0.611644
H	1.636657	-2.582198	0.690490
H	0.178351	-2.848677	1.664520
H	0.180768	-3.298996	-0.025762

6a S_0

Atom	x	y	z
C	0.801949	1.084224	-0.287662
C	1.346020	-0.151035	0.042297
C	0.501605	-1.216236	0.324830
C	-0.874481	-1.030545	0.273247
C	-1.412681	0.198739	-0.055123
C	-0.566642	1.265991	-0.338195
F	-1.670657	-2.073134	0.549848
F	1.016528	-2.404101	0.642133
F	2.667155	-0.321905	0.089840
F	1.636318	2.098556	-0.556640
H	-2.486261	0.311330	-0.086766
H	-0.958852	2.238115	-0.597808

6a T_1

Atom	x	y	z
C	0.813906	1.061897	-0.499344
C	1.429225	-0.188887	-0.019646
C	0.513380	-1.318366	0.131809
C	-0.807189	-1.067428	0.283456
C	-1.339937	0.239524	0.109519
C	-0.514551	1.291478	-0.348685
F	-1.670761	-2.065861	0.527618
F	1.015771	-2.557034	0.148808
F	2.261697	0.002179	1.049617
F	1.629964	1.961481	-1.057789
H	-2.391460	0.394244	0.298578
H	-0.940045	2.246773	-0.623940

7a S_0

Atom	x	y	z
C	1.231796	1.624206	-0.431139
C	0.651722	2.972210	-0.790887
O	2.429698	1.448991	-0.382831
C	0.288951	0.494361	-0.131524
C	0.836140	-0.745614	0.199786
C	-0.012511	-1.798647	0.479295
C	-1.395384	-1.668750	0.442680
C	-1.934788	-0.434987	0.112949
C	-1.099030	0.639336	-0.172220
N	0.567986	-3.112696	0.830455
O	-0.208767	-4.023575	1.072290
O	1.783033	-3.205301	0.856783
H	1.466004	3.667126	-0.974033
H	0.027108	2.899864	-1.683374
H	0.023477	3.352137	0.017106
H	1.907070	-0.870557	0.234649
H	-2.017019	-2.520829	0.668968
H	-3.007979	-0.310478	0.078174
H	-1.537512	1.593203	-0.427125

7a T_1

Atom	x	y	z
C	1.230726	1.629102	-0.432498
C	0.651607	2.977451	-0.792236
O	2.429181	1.454772	-0.384468
C	0.286959	0.499343	-0.132912
C	0.838188	-0.733785	0.196564
C	-0.012172	-1.803667	0.480575
C	-1.408225	-1.661649	0.440729
C	-1.937595	-0.428586	0.111219
C	-1.103122	0.650308	-0.175177
N	0.526450	-3.026962	0.807501
O	-0.121504	-4.108823	1.095273
O	1.784370	-3.326308	0.889191
H	1.466458	3.671795	-0.975223
H	0.026692	2.905043	-1.684383
H	0.023137	3.357078	0.015585
H	1.911688	-0.847941	0.228562
H	-2.041031	-2.507586	0.665375
H	-3.010895	-0.303272	0.076257
H	-1.540915	1.603688	-0.429931

1b S_0

Atom	x	y	z
C	-1.207002	-0.991741	1.023885
C	-2.290746	-1.042937	0.186620
C	-2.243109	-0.418556	-1.078609
C	-1.112700	0.244006	-1.480260
C	0.024088	0.315685	-0.639731
C	1.207002	0.991741	-1.023885
C	2.290746	1.042937	-0.186620
C	2.243109	0.418556	1.078609
C	1.112700	-0.244006	1.480260
C	-0.024089	-0.315685	0.639732
H	-1.241189	-1.469912	1.994857
H	-3.188788	-1.563016	0.492518
H	-3.105086	-0.465827	-1.730755
H	-1.073770	0.723730	-2.450286
H	1.241188	1.469912	-1.994856
H	3.188787	1.563016	-0.492519
H	3.105085	0.465827	1.730756
H	1.073770	-0.723730	2.450286

1b T_1

Atom	x	y	z
C	-1.200300	-0.988848	1.023637
C	-2.340361	-1.047222	0.152391
C	-2.294545	-0.446827	-1.064251
C	-1.106110	0.245380	-1.477393
C	0.024368	0.319349	-0.647136
C	1.200300	0.988847	-1.023636
C	2.340361	1.047222	-0.152391
C	2.294545	0.446827	1.064251
C	1.106110	-0.245380	1.477393
C	-0.024368	-0.319349	0.647136
H	-1.244064	-1.469743	1.991950
H	-3.227823	-1.572315	0.478004
H	-3.144617	-0.481850	-1.731697
H	-1.076827	0.721614	-2.448553
H	1.244063	1.469742	-1.991950
H	3.227822	1.572316	-0.478003
H	3.144616	0.481851	1.731698
H	1.076826	-0.721614	2.448553

2b S_0

Atom	x	y	z
C	1.914707	-0.508558	0.126832
C	2.946870	0.425012	0.064169
C	2.582007	1.763092	-0.093679
C	1.255189	2.143058	-0.183731
C	0.243908	1.190098	-0.118248
C	-1.170741	1.646892	-0.220376
O	-1.436787	2.826997	-0.357254
C	-2.233139	0.614166	-0.149492
C	-3.568461	1.004698	-0.242890
C	-4.575736	0.055418	-0.178982
C	-4.257415	-1.293069	-0.020994
C	-2.933055	-1.689580	0.072795
C	-1.913146	-0.740490	0.009269
C	-0.504375	-1.201535	0.113445
O	-0.234206	-2.377836	0.253360
C	0.566931	-0.166817	0.040309
C	4.387619	0.015056	0.161996
N	2.340120	-1.919369	0.293829
O	2.580582	-2.540878	-0.722831
O	2.507866	-2.307624	1.433471
H	3.361471	2.511620	-0.145732
H	0.975871	3.179447	-0.306039
H	-3.790786	2.055000	-0.364904
H	-5.610675	0.361312	-0.251796
H	-5.045592	-2.032144	0.028585
H	-2.663951	-2.728718	0.195561
H	4.649886	-0.682850	-0.634349
H	5.037914	0.883384	0.087290
H	4.587127	-0.485778	1.110386

2b T_1

Atom	x	y	z
C	1.900278	-0.540254	0.123788
C	2.932040	0.406067	0.085037
C	2.568581	1.742369	-0.087990
C	1.244177	2.119682	-0.203525
C	0.230191	1.166909	-0.162051
C	-1.178836	1.638035	-0.270535
O	-1.432013	2.819228	-0.423956
C	-2.251704	0.621204	-0.167786
C	-3.584543	1.029034	-0.209966
C	-4.600260	0.091821	-0.114005
C	-4.292074	-1.261759	0.019523
C	-2.970126	-1.675183	0.054977
C	-1.941116	-0.737642	-0.035081
C	-0.533996	-1.222579	-0.006151
O	-0.291422	-2.412529	0.007336
C	0.551917	-0.190523	-0.009115
C	4.373811	0.017544	0.216905
N	2.250050	-1.927902	0.325563
O	2.830391	-2.584565	-0.646062
O	2.882523	-2.264935	1.413956
H	3.347335	2.492446	-0.129430
H	0.965857	3.156182	-0.328716
H	-3.797770	2.082774	-0.317794
H	-5.633468	0.410510	-0.143719
H	-5.086579	-1.991946	0.093983
H	-2.709973	-2.719289	0.151246
H	4.622670	-0.797783	-0.461768
H	5.016853	0.867549	-0.001099
H	4.587206	-0.334457	1.226432

3b S_0

Atom	x	y	z
-1.156235	0.298448	-0.276643	
-2.237138	0.616916	-1.071845	
-2.086066	1.338775	-2.265758	
-0.841866	1.758500	-2.652008	
0.295129	1.486479	-1.857269	
1.571973	1.956361	-2.249196	
2.676710	1.725776	-1.475837	
2.542627	1.014501	-0.267579	
1.323190	0.536585	0.138637	
0.155813	0.742581	-0.640580	
-1.496534	-0.509347	0.934356	
-2.582451	-0.490094	1.464873	
-0.498643	-1.308348	1.356814	
-0.790527	-2.139920	2.501418	
0.457102	-2.932161	2.816130	
-3.216482	0.287411	-0.86526	
-2.953898	1.556732	-2.873060	
-0.708719	2.314970	-3.571261	
1.653900	2.511327	-3.175193	
3.647118	2.091681	-1.783390	
3.414129	0.842967	0.350459	
1.247784	-0.007619	1.063652	
-1.634887	-2.784150	2.256066	
-1.093390	-1.500322	3.330464	
0.272633	-3.584447	3.670598	
1.288707	-2.272246	3.064365	
0.80027	-3.551352	1.968317	

3b T_1

Atom	x	y	z
C	-1.143022	0.167981	-0.363631
C	-2.301028	0.657773	-1.112226
C	-2.164565	1.533842	-2.129926
C	-0.872209	2.010620	-2.506212
C	0.285073	1.573458	-1.819206
C	1.547558	2.043191	-2.190894
C	2.725477	1.628543	-1.527163
C	2.630186	0.743218	-0.492170
C	1.359241	0.248605	-0.092359
C	0.175293	0.635994	-0.724880
C	-1.493279	-0.775132	0.700932
O	-2.643189	-1.111878	0.932152
O	-0.457029	-1.261633	1.426642
C	-0.801120	-2.190211	2.473290
C	0.484866	-2.608056	3.149234
H	-3.266491	0.284626	-0.810988
H	-3.035799	1.881545	-2.668638
H	-0.764930	2.712225	-3.321736
H	1.616716	2.744888	-3.012091
H	3.684509	2.014909	-1.844478
H	3.512346	0.407382	0.034966
H	1.312341	-0.447065	0.725087
H	-1.326361	-3.038260	2.033362
H	-1.487390	-1.702200	3.165771
H	0.267162	-3.313749	3.951851
H	0.997009	-1.747734	3.581163
H	1.158639	-3.092880	2.442150

4b S_0

Atom	x	y	z
C	-1.172412	-0.975483	1.019983
C	-2.246400	-1.018424	0.173951
C	-2.214086	-0.399712	-1.092765
C	-1.081798	0.260584	-1.488045
C	0.056032	0.333665	-0.649537
C	1.237397	1.009602	-1.034766
C	2.321251	1.060735	-0.197260
C	2.272414	0.436131	1.067378
C	1.142808	-0.226946	1.470783
C	0.006754	-0.297791	0.629142
Cl	-3.702138	-1.854117	0.654416
H	-1.218554	-1.456673	1.986845
H	-3.081923	-0.454908	-1.733414
H	-1.048271	0.738419	-2.458827
H	1.271062	1.487531	-2.005676
H	3.219350	1.580592	-0.502621
H	3.134082	0.483145	1.719805
H	1.104431	-0.706346	2.440606

4b T_1

Atom	x	y	z
C	-1.162868	-0.969936	1.016650
C	-2.299195	-1.018338	0.127786
C	-2.266739	-0.423290	-1.089278
C	-1.080983	0.263182	-1.492752
C	0.056616	0.338554	-0.659238
C	1.226585	1.003844	-1.032118
C	2.366390	1.061670	-0.159929
C	2.321551	0.460803	1.058552
C	1.137931	-0.227882	1.468498
C	0.007452	-0.300122	0.634611
Cl	-3.708010	-1.868997	0.680450
H	-1.226595	-1.456242	1.978886
H	-3.121981	-0.465007	-1.747206
H	-1.053968	0.738427	-2.463811
H	1.273479	1.485722	-1.999758
H	3.253679	1.586771	-0.485692
H	3.171754	0.496124	1.725509
H	1.104898	-0.705281	2.438834

1c S_0

Atom	x	y	z
C	-0.012793	0.730249	-1.645404
C	0.897947	0.389769	-0.487732
C	2.257064	0.595859	-0.364005
C	2.911851	0.197516	0.813236
C	2.165199	-0.403641	1.841061
C	0.800200	-0.607140	1.708933
C	0.154559	-0.211719	0.542258
C	-1.244661	-0.295900	0.127366
C	-2.365577	-0.801244	0.778497
C	-3.598824	-0.81817	0.135128
C	-3.715294	-0.205936	-1.141153
C	-2.592627	0.301662	-1.796551
C	-1.364661	0.255172	-1.162067
N	4.265942	0.392702	0.959469
H	-0.010725	1.802321	-1.861464
H	0.292842	0.223119	-2.564867
H	2.824602	1.060374	-1.162329
H	2.670957	-0.710447	2.748399
H	0.249681	-1.072552	2.516492
H	-2.284888	-1.227323	1.770274
H	-4.477791	-1.141835	0.631635
H	-4.681603	-0.175484	-1.626669
H	-2.687519	0.725288	-2.788920
H	4.806482	0.819895	0.233325
H	4.739635	0.111108	1.795086

1c T_1

Atom	x	y	z
C	-0.003867	0.82883	-1.686274
C	0.912972	0.412500	-0.529273
C	2.239641	0.604126	-0.391525
C	2.892394	0.183241	0.834169
C	2.137833	-0.418746	1.863974
C	0.787443	-0.624581	1.747408
C	0.122317	-0.207604	0.523890
C	-1.201279	-0.286611	0.128783
C	-2.356671	-0.809731	0.803163
C	-3.572441	-0.760416	0.163024
C	-3.706379	-0.212944	-1.127213
C	-2.571782	0.309132	-1.807870
C	-1.354980	0.273743	-1.198121
N	4.242741	0.383097	0.964399
H	-0.003354	1.825282	-1.898955
H	0.301832	0.248297	-2.606590
H	2.832121	1.065116	-1.173419
H	2.652457	-0.722880	2.768614
H	0.226157	-1.086656	2.545594
H	-2.266682	-1.232840	1.794125
H	-4.452217	-1.151040	0.658960
H	-4.676744	-0.189410	-1.602588
H	-2.686286	0.727985	-2.800129
H	4.774015	0.811032	0.230236
H	4.730755	0.107020	1.795615

2c S_0

Atom	x	y	z
C	-2.116971	2.776438	0.537094
C	-0.983744	3.519618	0.509208
C	0.236825	2.947538	0.048650
C	0.291009	1.558988	-0.262003
C	-0.863091	0.722119	0.012891
C	-0.864965	-0.719553	-0.025152
C	0.282636	-1.559841	0.266043
C	0.228722	-2.948237	-0.045340
C	-0.986901	-3.516704	-0.523129
C	-2.117403	-2.770155	-0.567061
C	-2.095016	-1.374354	-0.275267
C	-3.313779	-0.652285	-0.197496
C	-3.314288	0.662133	0.150557
C	-2.094608	1.380576	0.245591
C	1.349856	-3.767105	0.210100
C	2.465530	-3.266590	0.833437
C	2.478550	-1.925029	1.249336
C	1.416194	-1.098639	0.972193
C	1.433067	1.094419	-0.952067
C	2.501693	1.917647	-1.214107
C	2.486782	3.259237	-0.798368
C	1.363893	3.763066	-0.190855
H	-3.068163	3.229603	0.785882
H	-1.004034	4.572823	0.88301
H	-1.006798	-4.569855	-0.772482
H	-3.066320	-3.220500	-0.829293
H	-4.242327	-1.183390	-0.362619
H	-4.243497	1.195999	0.302535
H	1.297205	-4.813236	-0.064199
H	3.313262	-3.907116	1.036634
H	3.325652	-1.538959	1.800446
H	1.443634	-0.077864	1.316690
H	1.462350	0.073564	-1.296179
H	3.355358	1.529061	-1.753192
H	3.339209	3.897238	-0.989513
H	1.310479	4.809347	0.082724

2c T_1

Atom	x	y	z
C	-2.137642	2.745154	0.464935
C	-0.940757	3.480864	0.529704
C	0.269518	2.907358	0.068733
C	0.291135	1.534886	-0.319106
C	-0.890498	0.692460	-0.050664
C	-0.893208	-0.689771	0.038208
C	0.281977	-1.535799	0.323436
C	0.262036	-2.907963	-0.065694
C	-0.943141	-3.477628	-0.544317
C	-2.139032	-2.738493	-0.495694
C	-2.156069	-1.401954	-0.167333
C	-3.393848	-0.660314	-0.116359
C	-3.393062	0.670339	0.069506
C	-2.153884	1.408299	0.137089
C	1.411071	-3.698629	0.146598
C	2.511833	-3.192509	0.810460
C	2.479799	-1.887240	1.299826
C	1.372981	-1.079633	1.059533
C	1.391557	1.075069	-1.038960
C	2.503865	1.879348	-1.263766
C	2.532478	3.185001	-0.774967
C	1.423709	3.694669	-0.127523
H	-3.076361	3.237557	0.685978
H	-0.956175	4.523113	0.817489
H	-0.957513	-4.519650	-0.832962
H	-3.075927	-3.228263	-0.729918
H	-4.321125	-1.210310	-0.214303
H	-4.319910	1.223152	0.154852
H	1.400597	-4.727928	-0.189030
H	3.380976	-3.815239	0.975254
H	3.315656	-1.495137	1.862930
H	1.367086	-0.070495	1.442375
H	1.388356	0.065710	-1.421226
H	3.346657	1.484540	-1.814512
H	3.405643	3.805174	-0.927703
H	1.411222	4.724267	0.207121

3c S_0			
Atom	x	y	z
C	2.140729	-1.766110	0.599104
C	3.349399	-1.603309	-0.010655
C	3.547669	-0.552869	-0.947422
C	2.531721	0.305375	-1.248191
C	1.252938	0.171573	-0.634427
C	0.195082	1.033558	-0.921683
C	-1.052147	0.892201	-0.314208
C	-2.140730	1.766110	-0.599105
C	-3.349399	1.603310	0.010655
C	-3.547669	0.552869	0.947422
C	-2.531721	-0.305375	1.248190
C	-1.252938	-0.171573	0.634426
C	-0.195082	-1.033559	0.921683
C	1.052147	-0.892201	0.314207
H	1.987874	-2.565776	1.312955
H	4.167045	-2.274672	0.215585
H	4.513518	-0.439080	-1.421388
H	2.680928	1.106144	-1.961571
H	0.346217	1.834407	-1.635832
H	-1.987874	2.565776	-1.312955
H	-4.167046	2.274672	-0.215585
H	-4.513518	0.439079	1.421388
H	-2.680929	-1.106144	1.961569
H	-0.346217	-1.834407	1.635831

3c T_1			
Atom	x	y	z
C	2.141956	-1.757743	0.591791
C	3.394505	-1.600206	-0.030998
C	3.586641	-0.582269	-0.938767
C	2.529827	0.297225	-1.240773
C	1.281255	0.161177	-0.637099
C	0.195475	1.035671	-0.923577
C	-1.081024	0.899674	-0.308937
C	-2.141957	1.757743	-0.591791
C	-3.394505	1.600207	0.030999
C	-3.586641	0.582269	0.938767
C	-2.529827	-0.297224	1.240772
C	-1.281255	-0.161177	0.637098
C	-0.195475	-1.035672	0.923575
C	1.081023	-0.899674	0.308936
H	1.994009	-2.558883	1.304919
H	4.200442	-2.280830	0.207425
H	4.545387	-0.453335	-1.422303
H	2.683929	1.096412	-1.954781
H	0.346514	1.836000	-1.637261
H	-1.994009	2.558883	-1.304919
H	-4.200441	2.280831	-0.207425
H	-4.545387	0.453335	1.422304
H	-2.683929	-1.096412	1.954780
H	-0.346515	-1.836002	1.637259

1d S_0

Atom	x	y	z
C	-0.462726	-0.575906	0.035381
C	-0.005831	-1.842195	0.414935
C	-0.873891	-2.923596	0.481614
C	-2.219104	-2.762164	0.169525
C	-2.687361	-1.509130	-0.209530
C	-1.818421	-0.428384	-0.275510
C	0.462623	0.575974	-0.035314
C	0.057476	1.849455	0.377496
C	0.925670	2.930791	0.311520
C	2.219183	2.762095	-0.169544
C	2.635635	1.501881	-0.583627
C	1.766657	0.421214	-0.516847
H	1.033960	-1.973284	0.682757
H	-0.500587	-3.892529	0.786167
H	-2.895819	-3.604531	0.221216
H	-3.730682	-1.374182	-0.462928
H	-2.188092	0.536838	-0.594519
H	-0.938930	1.986640	0.775545
H	0.593992	3.905495	0.644507
H	2.895992	3.604387	-0.221217
H	3.637396	1.361155	-0.967831
H	2.092861	-0.550021	-0.863794

1d T_1

Atom	x	y	z
C	-0.433287	-0.539992	0.032965
C	0.037704	-1.923849	0.011392
C	-0.826911	-2.974552	0.074979
C	-2.223712	-2.770646	0.165255
C	-2.721699	-1.446948	0.189529
C	-1.882900	-0.375426	0.127426
C	0.433303	0.539856	-0.031818
C	-0.037714	1.923865	-0.010812
C	0.826802	2.974505	-0.075826
C	2.223624	2.770707	-0.166683
C	2.721710	1.446938	-0.189567
C	1.883077	0.375432	-0.126179
H	1.094749	-2.123597	-0.056284
H	-0.438842	-3.984809	0.056205
H	-2.899228	-3.612249	0.215136
H	-3.789431	-1.283488	0.258798
H	-2.304067	0.616529	0.148901
H	-1.094690	2.123706	0.057618
H	0.438586	3.984722	-0.057641
H	2.899004	3.612308	-0.218256
H	3.789452	1.283453	-0.258643
H	2.304469	-0.616461	-0.146492

2d S_0

Atom	x	y	z
C	-0.464480	-0.573303	0.028387
C	-0.008278	-1.844693	0.396512
C	-0.873469	-2.924132	0.453332
C	-2.208859	-2.727198	0.134659
C	-2.695657	-1.482425	-0.235663
C	-1.819394	-0.411560	-0.284926
C	0.464224	0.573491	-0.028284
C	0.053661	1.846704	0.384558
C	0.919476	2.926037	0.335816
C	2.208930	2.727135	-0.134661
C	2.649597	1.480547	-0.553475
C	1.773646	0.409840	-0.496004
N	3.135750	3.871215	-0.191100
O	4.264837	3.664250	-0.607595
O	2.718019	4.956273	0.182126
N	-3.135474	-3.871454	0.191034
O	-4.305265	-3.666293	-0.092926
O	-2.676852	-4.954843	0.518258
H	1.028941	-1.984264	0.666179
H	-0.534046	-3.905448	0.745781
H	-3.739157	-1.370458	-0.485233
H	-2.185485	0.556719	-0.595463
H	-0.945323	1.987883	0.772027
H	0.616173	3.908783	0.661286
H	3.657121	1.367107	-0.921908
H	2.101364	-0.559910	-0.842713

2d T_1

Atom	x	y	z
C	-0.438863	-0.542117	0.026057
C	0.030890	-1.916507	-0.000379
C	-0.824603	-2.971034	0.051245
C	-2.216335	-2.738383	0.133539
C	-2.731280	-1.422399	0.162974
C	-1.878278	-0.365869	0.111199
C	0.438913	0.542247	-0.026764
C	-0.030841	1.916452	0.000570
C	0.824670	2.971034	-0.050808
C	2.216372	2.738374	-0.133041
C	2.731246	1.422440	-0.163491
C	1.878160	0.365883	-0.112600
N	3.120270	3.855156	-0.186991
O	4.326821	3.613005	-0.250170
O	2.634019	4.987196	-0.166762
N	-3.120255	-3.855196	0.188029
O	-4.325885	-3.613010	0.266629
O	-2.634849	-4.987238	0.152834
H	1.087150	-2.119225	-0.062425
H	-0.469531	-3.989231	0.031136
H	-3.799121	-1.284912	0.226364
H	-2.294687	0.627453	0.134665
H	-1.087062	2.119160	0.063300
H	0.469646	3.989243	-0.030471
H	3.799080	1.284963	-0.227025
H	2.294352	-0.627483	-0.137615

3d S_0

Atom	x	y	z
C	-0.464135	-0.576657	0.039590
C	-0.210847	-1.658046	0.886469
C	-1.071498	-2.743008	0.970714
C	-2.219440	-2.757949	0.191677
C	-2.505941	-1.702480	-0.662006
C	-1.629588	-0.628856	-0.728299
C	0.463982	0.576680	-0.040477
C	0.319665	1.687023	0.794422
C	1.181656	2.772279	0.729687
C	2.219589	2.757873	-0.190852
C	2.395921	1.673109	-1.037639
C	1.520592	0.599925	-0.953549
Cl	1.754028	-0.84738	-2.022799
Cl	-2.002255	0.688798	-1.804298
Cl	-0.978623	1.719012	1.954709
Cl	1.226415	-1.652782	1.869848
H	-0.838772	-3.558910	1.638321
H	-2.896354	-3.599127	0.250345
H	-3.396202	-1.703628	-1.272735
H	1.035203	3.611159	1.393300
H	2.896560	3.599058	-0.248746
H	3.200043	1.651263	-1.757686

3d T_1

Atom	x	y	z
C	-0.511239	-0.574402	0.021997
C	-0.183204	-1.653388	0.854793
C	-0.992613	-2.773457	0.984900
C	-2.177195	-2.836039	0.265682
C	-2.545123	-1.796180	-0.575928
C	-1.714030	-0.690618	-0.689183
C	0.370517	0.597022	-0.104603
C	0.226823	1.792880	0.652480
C	1.240117	2.770869	0.85151
C	2.470633	2.610873	0.085127
C	2.479539	1.635718	-0.935381
C	1.453396	0.669984	-1.021634
Cl	1.481331	-0.384744	-2.394905
Cl	-2.189167	0.590589	-1.771796
Cl	-1.285804	2.148317	1.413225
Cl	1.301520	-1.596517	1.768863
H	-0.694985	-3.577613	1.641162
H	-2.817169	-3.702739	0.359575
H	-3.461828	-1.837120	-1.144828
H	1.024655	3.664188	1.326924
H	3.281496	3.307581	0.211813
H	3.242329	1.634796	-1.703437

4d S_0

Atom	x	y	z
C	-0.515772	1.281537	0.107442
C	-1.394800	0.094577	0.160901
C	-0.966341	-1.080584	0.793219
C	-1.812372	-2.175452	0.899496
C	-3.088774	-2.126256	0.351332
C	-3.521293	-0.968925	-0.290755
C	-2.688013	0.134467	-0.374375
C	0.933895	1.050679	-0.064811
C	1.872148	1.892666	0.544436
C	3.229434	1.694051	0.351663
C	3.676581	0.665714	-0.473793
C	2.756092	-0.169429	-1.096185
C	1.396783	0.011065	-0.882910
S	-1.127463	2.801537	0.234751
H	0.023295	-1.123102	1.224519
H	-1.474141	-3.067255	1.409927
H	-3.743882	-2.984243	0.423403
H	-4.511449	-0.927944	-0.724519
H	-3.020769	1.041426	-0.858130
H	1.516191	2.697161	1.171663
H	3.941999	2.342704	0.843332
H	4.736747	0.517210	-0.630298
H	3.096182	-0.962937	-1.748055
H	0.685722	-0.638670	-1.372252

4d T_1

Atom	x	y	z
C	-0.453583	1.121430	0.130928
C	-1.386625	0.015553	0.161260
C	-0.996489	-1.247807	0.654176
C	-1.899044	-2.293305	0.722776
C	-3.222370	-2.117934	0.318045
C	-3.629564	-0.875966	-0.158382
C	-2.730469	0.174806	-0.238982
C	0.977608	0.995683	-0.043018
C	1.870558	1.951955	0.485848
C	3.235308	1.851432	0.270678
C	3.756618	0.797156	-0.472327
C	2.889233	-0.155468	-1.007035
C	1.524634	-0.058599	-0.804932
S	-1.097904	2.714509	0.316133
H	0.015870	-1.388898	1.003720
H	-1.574826	-3.251283	1.107919
H	-3.924237	-2.938578	0.376356
H	-4.651585	-0.728588	-0.481867
H	-3.049182	1.124752	-0.646063
H	1.480449	2.754850	1.096487
H	3.897792	2.593370	0.696742
H	4.822617	0.717446	-0.635922
H	3.282575	-0.972183	-1.598163
H	0.862618	-0.784332	-1.254375

1e S_0

Atom	x	y	z
N	1.732739	0.973610	0.017180
C	1.303989	2.145298	0.420216
C	-0.048276	2.436513	0.709847
C	-0.980246	1.445289	0.565791
C	-0.568170	0.165147	0.134028
C	-1.460115	-0.918309	-0.042696
C	-0.997251	-2.137210	-0.464508
C	0.377480	-2.325415	-0.727884
C	1.266653	-1.294940	-0.566031
C	0.820336	-0.025101	-0.132011
H	2.053484	2.922730	0.530382
H	-0.325853	3.428673	1.038130
H	-2.027326	1.624734	0.776773
H	-2.513125	-0.768015	0.160800
H	-1.684338	-2.962066	-0.597812
H	0.727178	-3.293816	-1.060281
H	2.322838	-1.417119	-0.761922

1e T_1

Atom	x	y	z
N	1.727872	0.961095	0.014327
C	1.289246	2.196227	0.437153
C	-0.013494	2.475363	0.715741
C	-0.990332	1.448348	0.568200
C	-0.582532	0.181487	0.140952
C	-1.454901	-0.909007	-0.040765
C	-0.973691	-2.198499	-0.485769
C	0.343763	-2.380222	-0.738584
C	1.262267	-1.287750	-0.563283
C	0.823198	-0.008583	-0.127658
H	2.059619	2.949572	0.537201
H	-0.303582	3.463551	1.044756
H	-2.032694	1.641837	0.782484
H	-2.510582	-0.777477	0.157731
H	-1.681139	-3.006438	-0.611105
H	0.719416	-3.337564	-1.071759
H	2.317564	-1.411937	-0.759621

S2 CDCB Optimized Geometries

The following tables report the cartesian coordinates in Å of optimized geometries of states S_0 and T_1 of compounds 2CzPN and 4CzIPN. Geometry optimizations have been performed at DFT level of theory, by employing B3LYP functional, D3BJ dispersion correction, def2-TZVPP basis set and RIJK approximation of ORCA 5.0.1.

2CzPN S_0

Atom	x	y	z
C	-2.346893	0.870413	1.376379
C	-3.466327	0.053564	1.494595
C	-3.453725	-1.223208	0.89863
C	-2.312569	-1.648735	0.227358
C	-1.183186	-0.841387	0.123541
C	-1.208205	0.453798	0.691636
C	-4.612688	0.52763	2.198372
C	-4.57929	-2.094137	0.991332
N	-0.119879	1.329972	0.595048
N	-0.057846	-1.339898	-0.5445
C	-0.040399	-1.763681	-1.883211
C	1.298871	-2.001883	-2.262018
C	2.12425	-1.726257	-1.105574
C	1.258826	-1.332472	-0.063117
C	0.576312	1.867193	1.69082

C	1.737311	2.51328	1.213292
C	1.739399	2.376907	-0.227303
C	0.579689	1.653248	-0.576875
C	0.246132	1.398141	-1.899061
C	1.128531	1.82901	-2.880101
C	2.300217	2.518649	-2.551409
C	2.605397	2.8075	-1.229141
C	0.298178	1.773719	3.048213
C	1.198477	2.355227	3.933464
C	2.34704	3.00931	3.477592
C	2.623149	3.089033	2.119894
C	1.727122	-1.053586	1.212622
C	3.097793	-1.113991	1.422398
C	3.975417	-1.46871	0.392606
C	3.495251	-1.788589	-0.86927
C	-1.089401	-1.891016	-2.784361
C	-0.781554	-2.282806	-4.081976
C	0.537487	-2.534337	-4.471557
C	1.581303	-2.39278	-3.567986
N	-5.526466	0.927193	2.774723
N	-5.476744	-2.813862	1.049201
H	-2.368434	1.865408	1.794595
H	-2.28248	-2.642375	-0.193513
H	-0.660028	0.878051	-2.167705
H	0.900654	1.624791	-3.917088
H	2.967536	2.839578	-3.339276
H	3.501763	3.359188	-0.979633
H	-0.578658	1.260949	3.416072
H	1.002658	2.298401	4.995456
H	3.026128	3.453393	4.192099
H	3.519053	3.583883	1.769636
H	1.060169	-0.789177	2.01813
H	3.489577	-0.881332	2.402895
H	5.038212	-1.504752	0.588023
H	4.174638	-2.083014	-1.657829
H	-2.111966	-1.68782	-2.500934
H	-1.581088	-2.39406	-4.801546
H	0.743567	-2.838989	-5.488226
H	2.602226	-2.574924	-3.875786

2CzPN T_1

Atom	x	y	z
C	-2.341129	0.856042	1.470342
C	-3.486072	0.063139	1.571596

C	-3.513796	-1.243408	0.853628
C	-2.374788	-1.643009	0.152881
C	-1.2384	-0.866577	0.097092
C	-1.239068	0.463052	0.743628
C	-4.595998	0.514644	2.295305
C	-4.630856	-2.084696	0.918963
N	-0.137518	1.313215	0.592009
N	-0.078902	-1.337758	-0.529256
C	0.01526	-1.728057	-1.868123
C	1.379012	-1.914706	-2.194748
C	2.14202	-1.654336	-0.989609
C	1.211143	-1.32613	0.018933
C	0.621929	1.844366	1.63907
C	1.781832	2.449439	1.101255
C	1.705511	2.304353	-0.339154
C	0.502156	1.621518	-0.617077
C	0.069978	1.395695	-1.917176
C	0.907005	1.794991	-2.951465
C	2.121818	2.435023	-2.693251
C	2.520957	2.708228	-1.388461
C	0.409711	1.756979	3.01108
C	1.371065	2.308577	3.847234
C	2.516249	2.923438	3.330103
C	2.730767	2.991757	1.957999
C	1.599029	-1.109535	1.334351
C	2.958468	-1.14567	1.617839
C	3.897836	-1.426058	0.622168
C	3.495762	-1.698084	-0.68202
C	-0.990352	-1.845492	-2.822218
C	-0.613348	-2.179137	-4.115974
C	0.729784	-2.380692	-4.451495
C	1.73157	-2.244414	-3.496833
N	-5.510078	0.896153	2.901012
N	-5.55092	-2.791378	0.96215
H	-2.344706	1.833769	1.930774
H	-2.364509	-2.620027	-0.308884
H	-0.881314	0.929738	-2.122458
H	0.605016	1.610531	-3.972891
H	2.7498	2.737298	-3.519743
H	3.447819	3.231742	-1.196823
H	-0.466055	1.27244	3.416048
H	1.229131	2.259955	4.917921
H	3.245579	3.344429	4.008183
H	3.628695	3.449256	1.565284

H	0.874598	-0.921465	2.111495
H	3.290169	-0.958916	2.629606
H	4.948862	-1.450224	0.874347
H	4.225773	-1.946245	-1.440518
H	-2.027438	-1.679087	-2.571782
H	-1.374486	-2.283761	-4.87664
H	0.990272	-2.640024	-5.468265
H	2.769664	-2.381226	-3.767806

4CzIPN S_0

Atom	x	y	z
C	2.288966	-0.005068	-0.000333
C	1.583489	1.056299	0.578531
C	0.176383	1.048544	0.617739
C	-0.537664	0.000825	0.000572
C	0.171603	-1.050004	-0.616867
C	1.578699	-1.063621	-0.578508
N	3.686393	-0.007855	-0.001088
N	-1.938547	0.003999	0.000538
N	-0.483171	2.107804	1.249016
N	-0.492835	-2.106511	-1.247597
C	2.297731	2.203921	1.030143
C	2.287890	-2.214341	-1.030187
C	-2.757556	0.013551	-1.137904
C	-4.105938	0.012540	-0.723312
C	-4.106168	0.007006	0.723726
C	-2.757938	-0.001258	1.138726
C	-1.510934	2.891784	0.699907
C	-2.099690	3.652342	1.730689
C	-1.397736	3.328282	2.954611
C	-0.402881	2.383997	2.627879
C	-1.524241	-2.885371	-0.697991
C	-0.414244	-2.383539	-2.626424
C	-1.413647	-3.323211	-2.952560
C	-2.116843	-3.643490	-1.728359
C	5.851533	-0.048059	0.720823
C	4.503211	-0.063484	1.136349
C	4.502065	0.044462	-1.139510
C	5.850813	0.023400	-0.725620
C	-1.552280	3.728200	4.279100
C	-0.725182	3.181807	5.250114
C	0.248675	2.238841	4.908278
C	0.421651	1.825488	3.593337
C	-3.149148	4.516028	1.427889

C	-3.585189	4.609427	0.113936
C	-2.966349	3.869947	-0.899189
C	-1.911849	3.011081	-0.621457
C	-5.115316	0.039706	-1.682007
C	-4.769370	0.074228	-3.025495
C	-3.426698	0.100489	-3.415630
C	-2.404078	0.080424	-2.476905
C	-5.115965	-0.014575	1.682125
C	-4.770617	-0.050791	3.025722
C	-3.428220	-0.084267	3.416265
C	-2.405236	-0.069872	2.477842
C	0.412684	-1.829312	-3.592301
C	0.237447	-2.242359	-4.907036
C	-0.740926	-3.180852	-5.248267
C	-1.570413	-3.722901	-4.276859
C	-1.925461	-3.002254	0.623491
C	-2.983980	-3.855979	0.901782
C	-3.606520	-4.592926	-0.110925
C	-3.170309	-4.502090	-1.425002
C	4.141253	0.143196	-2.475118
C	5.162654	0.200161	-3.413952
C	6.506302	0.167254	-3.026531
C	6.857250	0.083861	-1.686729
C	4.143596	-0.160605	2.472395
C	5.165892	-0.221763	3.409994
C	6.509192	-0.194510	3.020945
C	6.858871	-0.112658	1.680717
N	2.878615	3.138035	1.369803
N	2.864595	-3.150998	-1.369966
H	-2.313294	4.448554	4.547525
H	-0.832918	3.486156	6.281968
H	0.885472	1.825159	5.678084
H	1.178431	1.097190	3.343592
H	-3.615305	5.105957	2.205478
H	-4.404826	5.269500	-0.134183
H	-3.312744	3.963873	-1.919028
H	-1.434680	2.453647	-1.412028
H	-6.154733	0.038883	-1.382226
H	-5.543772	0.088609	-3.779939
H	-3.173853	0.134541	-4.466336
H	-1.373225	0.111598	-2.792394
H	-6.155272	-0.008120	1.382034
H	-5.545310	-0.060849	3.779937
H	-3.175875	-0.119478	4.467054

H	-1.374655	-0.106424	2.793634
H	1.172969	-1.104518	-3.343050
H	0.876025	-1.832008	-5.677147
H	-0.850336	-3.485092	-6.279977
H	-2.334921	-4.439712	-4.544835
H	-1.445498	-2.446775	1.413744
H	-3.330606	-3.947852	1.921730
H	-4.429241	-5.248989	0.137620
H	-3.639431	-5.090092	-2.202269
H	3.105272	0.177067	-2.780301
H	4.912027	0.271292	-4.463446
H	7.278419	0.212103	-3.781977
H	7.897921	0.069525	-1.391865
H	3.107847	-0.190097	2.778811
H	4.916246	-0.291752	4.459798
H	7.282030	-0.242540	3.775458
H	7.899237	-0.102668	1.384596

4CzIPN T_1

Atom	x	y	z
C	2.299609	-0.004649	-0.000854
C	1.619331	1.050437	0.626065
C	0.170841	1.026113	0.661516
C	-0.513942	0.001138	0.000021
C	0.166206	-1.026698	-0.661791
C	1.614614	-1.056971	-0.627339
N	3.701436	-0.007580	-0.001215
N	-1.925222	0.004170	0.000241
N	-0.527956	2.079058	1.281420
N	-0.537367	-2.076871	-1.280985
C	2.311023	2.185034	1.091948
C	2.301355	-2.194340	-1.093723
C	-2.738818	0.070453	-1.132303
C	-4.091179	0.050626	-0.723413
C	-4.091195	-0.030518	0.724507
C	-2.738842	-0.057693	1.133000
C	-1.430621	2.949638	0.660930
C	-2.074635	3.725329	1.650639
C	-1.509690	3.328880	2.924676
C	-0.550999	2.324552	2.650383
C	-1.443196	-2.943522	-0.659589
C	-0.562379	-2.322692	-2.649855
C	-1.525542	-3.323006	-2.923170

C	-2.091161	-3.716782	-1.648610
C	5.867011	-0.012606	0.723588
C	4.516113	-0.003790	1.135191
C	4.515582	-0.015341	-1.137968
C	5.866689	-0.013195	-0.726963
C	-1.737721	3.711017	4.241321
C	-1.014909	3.094942	5.256493
C	-0.068044	2.104393	4.966798
C	0.177298	1.705846	3.661790
C	-3.033100	4.658207	1.270035
C	-3.328763	4.808285	-0.080603
C	-2.662206	4.049964	-1.047350
C	-1.697385	3.116200	-0.690437
C	-5.094178	0.135943	-1.679424
C	-4.739530	0.244752	-3.021205
C	-3.397267	0.293086	-3.405424
C	-2.378454	0.220456	-2.465090
C	-5.094342	-0.110240	1.680840
C	-4.739873	-0.220792	3.022532
C	-3.397772	-0.276396	3.406355
C	-2.378877	-0.209454	2.465693
C	0.167832	-1.707407	-3.661968
C	-0.080189	-2.105236	-4.966683
C	-1.031530	-3.091770	-5.255416
C	-1.756206	-3.704488	-4.239544
C	-1.709505	-3.108768	0.692030
C	-2.677734	-4.038625	1.049921
C	-3.348133	-4.794447	0.083877
C	-3.053003	-4.645781	-1.267034
C	4.153209	0.023842	-2.477889
C	5.173235	0.039723	-3.419028
C	6.516099	0.027224	-3.031531
C	6.870651	0.006522	-1.686263
C	4.154141	-0.041290	2.475265
C	5.174493	-0.062318	3.415956
C	6.517228	-0.056469	3.027870
C	6.871285	-0.037400	1.682446
N	2.856776	3.121727	1.499220
N	2.843054	-3.133205	-1.501414
H	-2.469531	4.472769	4.474666
H	-1.180575	3.386281	6.284521
H	0.487339	1.647084	5.774085
H	0.912231	0.947960	3.434317
H	-3.538943	5.261632	2.011941

H	-4.074860	5.527426	-0.389187
H	-2.897208	4.191620	-2.093229
H	-1.170539	2.545173	-1.439167
H	-6.135454	0.126000	-1.386964
H	-5.511821	0.305052	-3.775474
H	-3.141099	0.389078	-4.451245
H	-1.344817	0.279122	-2.764175
H	-6.135639	-0.094583	1.388707
H	-5.512249	-0.276715	3.777049
H	-3.141813	-0.373581	4.452115
H	-1.345467	-0.273559	2.764464
H	0.906168	-0.952616	-3.435236
H	0.476536	-1.650509	-5.774503
H	-1.199232	-3.382635	-6.283248
H	-2.491468	-4.463135	-4.472149
H	-1.179698	-2.539775	1.440220
H	-2.912417	-4.179168	2.096022
H	-4.096834	-5.510546	0.393224
H	-3.561851	-5.247340	-2.008402
H	3.116372	0.033155	-2.776873
H	4.921860	0.059259	-4.470348
H	7.288245	0.038451	-3.788257
H	7.911914	0.010937	-1.393585
H	3.117405	-0.045578	2.774699
H	4.923484	-0.080733	4.467383
H	7.289645	-0.071641	3.784251
H	7.912384	-0.047006	1.389309

S3 Basis Set Convergence Plots

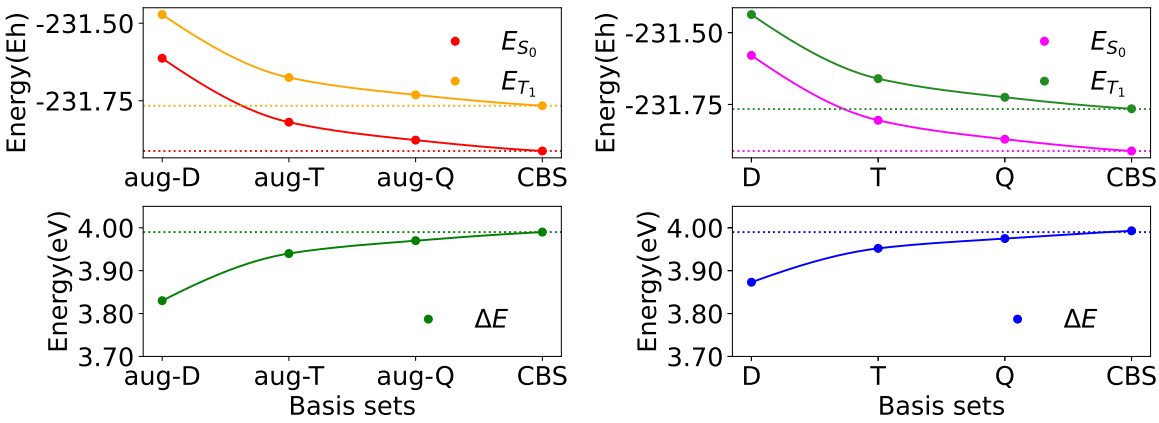

Figure S1: Basis set convergence of singlet state (E_{S_0}), triplet state (E_{T_1}) and ΔE gap of compound **1a** (Figure 1) for basis sets family aug-cc-pVNZ (N=D,T,Q) (Figure (A)) and for basis sets family cc-pVNZ (N=D,T,Q) (Figure (B)). Horizontal dotted lines represent energies extrapolated by means of Equation 2a and Equation 2b.

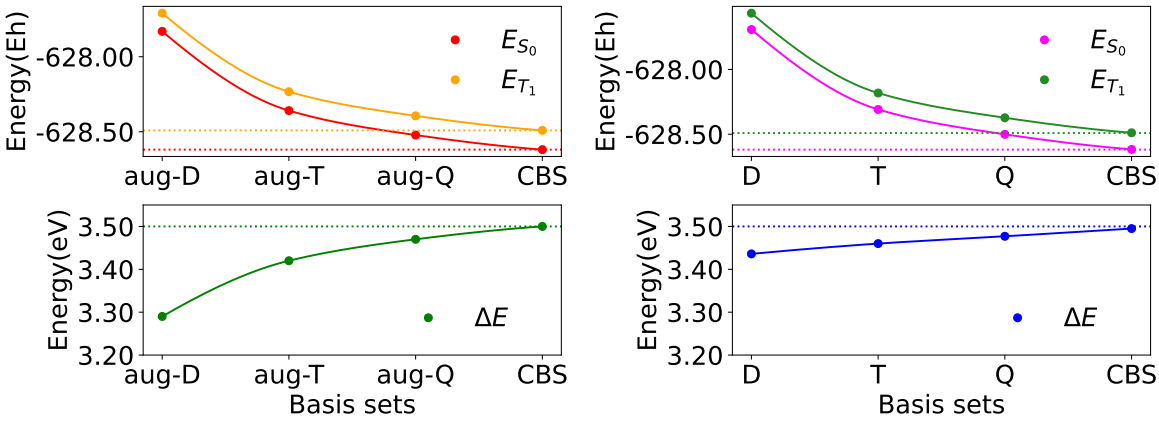

Figure S2: Basis set convergence of singlet state (E_{S_0}), triplet state (E_{T_1}) and ΔE gap of compound **6a** (Figure 1) for basis sets family aug-cc-pVNZ (N=D,T,Q) (Figure (A)) and for basis sets family cc-pVNZ (N=D,T,Q) (Figure (B)). Horizontal dotted lines represent energies extrapolated by means of Equation 2a and Equation 2b.