Supplementary Material (ESI) for PCCP

Supporting Information:

Carbazole Endcapped Heterofluorenes as Host Materials: Theoretical Study of Their Structural, Electronic, and Optical Properties

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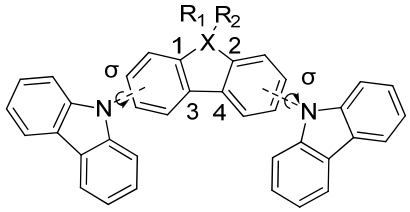
Table S1. The total energies and relative stability of Anti- and Syn- Configurations of CzCFs.

Molecule	E_{Anti} (a.u.)	E_{Syn} (a.u.)	$E_{(Anti-Syn)}$ (kcal/mol)
m-CzCF	-1612.595571	-1612.595584	0.00762
p-CzCF	-1612.596277	-1612.596279	0.00132
m-CzSiF	-1864.008959	-1864.008865	-0.05890
p-CzSiF	-1864.009218	-1864.009194	-0.01510
m-CzGeF	-3649.509260	-3649.509117	-0.08985
p-CzGeF	-3649.510110	-3649.510086	-0.01515
m-CzNF	-1589.326684	-1589.326659	-0.01613
p-CzNF	-1589.327562	-1589.327476	-0.05410
m-CzPF	-1875.923114	-1875.923035	-0.04898
p-CzPF	-1875.923343	-1875.923217	-0.07939
m-CzOF	-1569.871676	-1569.871592	-0.05292
p-CzOF	-1569.872188	-1569.872171	-0.01066
m-CzSF	-1892.849913	-1892.849899	-0.00882
p-CzSF	-1892.850409	-1892.850327	-0.05136

The stability of the anti and syn configuration is almost equivalent within 0.1kcal/mol as seen in Table S1. For most of CzCFs, the anti configuration is much more stable than the anti configuration, so the former configuration is more suitable to the following calculations.

Table S2. Central Hetero-ring and Inter-ring Bond Lengths (Å), Bond Angles (º), Dihedral Angles (º) and Dipole Moment (μ) of CzHFs in the Ground-State.



Molecules	Central hetero-ring						Inter-ring		Dipole Moment (μ)
	Bond Lengths			Bond Angles			Bond Lengths	Torsion Angles	
	X−C(1)	C(1)−C(3)	C(3)−C(4)	X−C(1)−C(3)	C(1)−C(3)−C(4)	C(1)−X−C(2)	C-N	σ	
m-CBP	—	1.4048	1.4868	—	120.75	—	1.420	55.8	2.5404
p-CBP	—	1.4055	1.4828	—	121.15	—	1.418	53.8	0.0003
m-CF	1.5279	1.4087	1.4689	111.06	108.41	101.06	1.421	56.7	3.0632
p-CF	1.5289	1.4094	1.4661	110.98	108.50	101.05	1.420	55.4	0.0972
m-SiF	1.8857	1.4185	1.48943	109.39	115.07	91.08	1.420	55.0	3.1472
p-SiF	1.8874	1.4190	1.4858	109.26	115.21	91.07	1.420	54.3	0.4306
m-GeF	1.9399	1.4152	1.49012	109.05	116.11	89.68	1.420	55.5	3.2993
p-GeF	1.9421	1.4156	1.48613	108.99	116.21	89.59	1.420	55.2	0.5281
m-NF	1.3890	1.4207	1.44752	109.16	106.53	108.60	1.423	61.0	4.7909
p-NF	1.3895	1.4211	1.4458	109.13	106.57	108.58	1.422	56.7	0.9717
m-PF	1.8388	1.4139	1.47201	112.33	113.04	89.04	1.420	55.1	2.2590
p-PF	1.8409	1.4144	1.46865	112.17	113.18	89.05	1.419	55.4	1.2786
m-OF	1.3757	1.4077	1.45211	111.72	105.32	105.91	1.422	59.2	1.6113
p-OF	1.3763	1.4081	1.45012	111.65	105.39	105.93	1.418	54.5	1.4888
m-SF	1.7662	1.4130	1.45503	112.51	112.06	90.85	1.420	57.4	1.6262
p-SF	1.7678	1.4135	1.45250	112.40	112.16	90.88	1.418	54.7	1.2328

The main geometric changes take places as follows: (1) After connecting the biphenyl of m-/p-CBPs with different bridging heteroatoms, the C(1)−C(3) bond lengths are predicted to be slightly lengthened in all the studied molecules with the maximum increase of 0.016 Å found in m-/p-CzNFs. (2) The adoption of Ge atom in m-/p-CzGeFs leads to the longest X−C(1) and C(3)−C(4) bond lengths, while the use of O atom in m-/p-CzOFs leads to the shortest ones; (3) In comparison with m-/p-CBPs, the C(3)−C(4) between the central biphenyl of CzHFs were predicted to be enhanced with reduced bond lengths (except for m-/p-CzSiFs and m-/p-CzGeFs), and the largest bond lengths decrement was 0.037 Å in m-/p-CzNFs, which may be ascribed to the different interactions between the heteroatoms and the adjacent carbons; (4) The largest five-membered hetero-ring was found in GeFs due to larger X−C(1), C(1)−C(3), and C(3)−C(4); (5) The average inter-ring bond length between heterofluorene and carbazole moiety at 3,6- or 2,7- positions is 1.420 Å and the torsion angles vary from 53º to 61º, indicating that the using of different bridging heteroatoms may influence the degree of spatial torsion of carbazole; (6) The p-type CzHFs have slightly better coplanar nature than m-type CzHFs with the lower torsion angle between the heterofluorene core and the carbazole substituents.

Table S3. Central Hetero-ring and Inter-ring Bond Lengths (Å), Bond Angles (º), Torsion Angles (º), and Dipole Moment (μ) of CzHFs in the lowest Triplet State (T_1)

Molecules	Central hetero-ring						Inter-ring		Dipole Moment (μ)
	Bond Lengths			Bond Angles			Bond Lengths	Torsion Angles	
	X−C(1)	C(1)−C(3)	C(3)−C(4)	X−C(1)−C(3)	C(1)−C(3)−C(4)	C(1)−X−C(2)	C-N	σ_1/σ_2	
m-CBP	—	1.4591	1.4025	—	122.63	—	1.405	51.8/51.8	1.2858
p-CBP	—	1.4667	1.4030	—	122.16	—	1.418	47.3/47.3	0.0104
m-CzCF	1.5301	1.4658	1.3875	110.25	109.34	100.82	1.417	50.5/50.5	1.6476
p-CzCF	1.5314	1.4574	1.3881	109.91	109.56	101.05	1.407	48.9/48.9	0.1757
m-CzSiF	1.8788	1.4821	1.4012	109.67	115.19	90.26	1.416	50.2/50.7	1.3125
p-CzSiF	1.8811	1.4765	1.3983	109.18	115.56	90.52	1.407	47.8/48.0	0.0607
m-CzGeF	1.9349	1.4782	1.4005	108.95	116.45	89.20	1.416	50.6/50.9	1.5594
p-CzGeF	1.9366	1.4713	1.3986	108.54	116.77	89.38	1.406	48.1/48.1	0.1784
m-CzNF	1.3940	1.4298	1.4206	107.96	107.19	110.02	1.415	47.7/45.8	2.7346
p-CzNF	1.3916	1.4562	1.3836	107.69	107.70	109.19	1.407	48.4/48.7	1.4179
m-CzPF	1.8411	1.4736	1.3909	112.42	113.42	88.19	1.416	50.7/50.6	0.9946
p-CzPF	1.8432	1.4660	1.3898	111.90	113.81	88.56	1.406	48.0/48.0	1.4018
m-CzOF	1.3886	1.4432	1.3861	110.45	106.63	106.36	1.423	55.6/49.0	3.2340
p-CzOF	1.3799	1.4440	1.3862	110.27	106.56	106.35	1.405	47.7/47.7	0.6939
m-CzSF	1.7504	1.4839	1.4028	110.79	112.90	91.79	1.404	43.2/57.8	4.2588
p-CzSF	1.7784	1.4530	1.3857	111.03	113.40	91.13	1.404	47.7/47.7	0.9033

Table S4. Molecular Orbital Compositions (%) in CzHFs

Molecules	Orbital	Biphenyl	Heteroatom	Methyl	Carbazole
m-CBP	LUMO	93.1	—	—	6.90
	HOMO	12.6	—	—	87.4
p-CBP	LUMO	87.9	—	—	12.1
	HOMO	20.8	—	—	79.2
m-CzCF	LUMO	89.3	0.70	4.00	6.00
	HOMO	14.9	0.20	0.30	84.6
p-CzCF	LUMO	84.0	0.60	3.80	11.6
	HOMO	24.0	0.10	0.10	75.8
m-CzSiF	LUMO	77.6	5.00	10.5	6.90
	HOMO	15.0	0.10	0.10	84.8
p-CzSiF	LUMO	76.5	4.63	9.59	9.28
	HOMO	23.3	0.13	0.07	76.5
m-CzGeF	LUMO	80.8	3.45	9.01	6.74
	HOMO	14.5	0.06	0.04	85.4
p-CzGeF	LUMO	78.4	3.24	8.16	10.2
	HOMO	23.1	0.30	0.10	76.5
m-CzNF	LUMO	92.9	1.00	1.00	5.10
	HOMO	19.1	6.30	1.10	73.5
p-CzNF	LUMO	86.6	0.90	0.90	11.6
	HOMO	24.1	0.10	0.00	75.8
m-CzPF	LUMO	77.2	5.20	11.8	5.80
	HOMO	12.5	3.20	1.80	82.5
p-CzPF	LUMO	74.9	4.80	10.6	9.70
	HOMO	21.2	0.20	0.10	78.5
m-CzOF	LUMO	93.6	0.90	—	5.50
	HOMO	12.9	2.10	—	85.0
p-CzOF	LUMO	87.6	0.90	—	11.5
	HOMO	21.2	0.10	—	78.7
m-CzSF	LUMO	92.2	2.16	—	5.64
	HOMO	14.7	6.30	—	79.0
p-CzSF	LUMO	86.3	2.10	—	11.6
	HOMO	20.8	0.10	—	79.1

Figue S1. The simulated absorption spectra of CzHFs in vacuum.

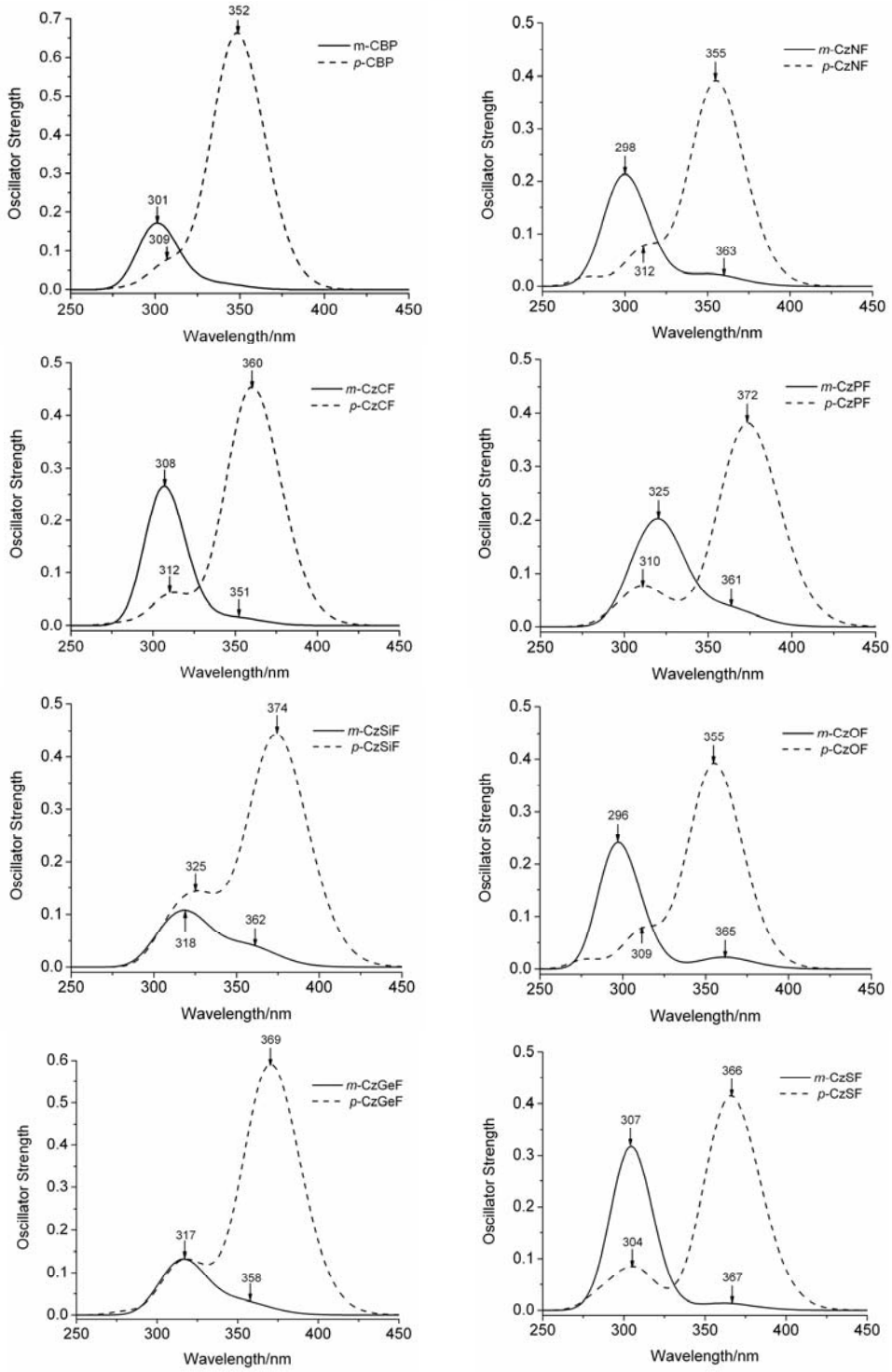


Table S5. Optimized geometries (in Å) and energies (in hartree) of *m*-CBP in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1495.85008			Energy = -1495.741359		
C	-2.71910100	3.64635000	0.95270300	2.83597300	3.85778900	0.33978800
C	-3.49223200	2.51579800	0.69392500	3.56068100	2.65097100	0.38143000
C	-2.88223200	1.36960400	0.16913300	2.83969100	1.41627100	0.26011900
C	-1.50943100	1.37030600	-0.09864300	1.47678200	1.40402300	0.11407700
C	-0.72876700	2.51151200	0.14021300	0.69685800	2.62795100	0.08021400
C	-1.35332400	3.65043900	0.67511200	1.46910400	3.86930200	0.19739700
C	0.72885600	2.51083700	-0.15278000	-0.69690900	2.62781600	-0.08072600
C	1.50955300	1.37079800	0.09149700	-1.47664000	1.40375300	-0.11452900
C	2.88239900	1.36893800	-0.17599800	-2.83950000	1.41585300	-0.26054500
C	3.49246900	2.51272800	-0.70590900	-3.56074700	2.65048200	-0.38197600
C	2.71932400	3.64205300	-0.97000300	-2.83624600	3.85742600	-0.34037500
C	1.35348100	3.64731700	-0.69276500	-1.46938300	3.86911000	-0.19800900
C	-3.15395400	-0.13242000	-2.55686700	2.30159100	-1.02154200	2.15442300
C	-3.43716800	-0.95271900	-3.64698800	2.29031300	-2.19407600	2.90733300
C	-4.29738000	-2.05784500	-3.52919100	3.25400200	-3.19811700	2.71503700
C	-4.89970400	-2.35869200	-2.31116100	4.26010600	-3.04004100	1.76560200
C	-4.63279500	-1.55055500	-1.19984100	4.29550700	-1.87069000	0.99880500
C	-3.75117500	-0.44770900	-1.33322300	3.30605500	-0.87389500	1.19412500
C	-5.08918500	-1.56061100	0.17437200	5.19015600	-1.38101700	-0.03036000
C	-5.94442300	-2.39653900	0.90175700	6.32291100	-1.91134400	-0.65558900
C	-6.16381100	-2.13453200	2.25096200	6.95464400	-1.17340700	-1.65412700
C	-5.53047700	-1.04898100	2.88011500	6.45560600	0.08186100	-2.03975700
C	-4.67540100	-0.20087800	2.17942900	5.32576800	0.63082100	-1.43589000
C	-4.46961500	-0.46146100	0.82174800	4.71088000	-0.10376300	-0.41716400
N	-3.65686600	0.20988600	-0.10003000	3.56888000	0.20247800	0.33281000
C	4.67429100	-0.21266100	-2.17890000	-5.32561600	0.63143800	1.43530100
C	5.52886600	-1.06467400	-2.87544700	-6.45561700	0.08293900	2.03926800
C	6.16221800	-2.14703000	-2.24083300	-6.95497200	-1.17228200	1.65390500
C	5.94337100	-2.40183100	-0.89016300	-6.32318700	-1.91083900	0.65584500
C	5.08868700	-1.56182600	-0.16683500	-5.19029700	-1.38098400	0.03049500
C	4.46910000	-0.46595600	-0.81975100	-4.71090100	-0.10364800	0.41684800
C	4.63304100	-1.54429500	1.20754800	-4.29552600	-1.87121900	-0.99831500
C	4.90034400	-2.34651500	2.32305800	-4.26021200	-3.04084700	-1.76468300
C	4.29863600	-2.03905100	3.53973400	-3.25388700	-3.19949400	-2.71379400
C	3.43860600	-0.93320500	3.65199700	-2.28999600	-2.19568700	-2.90628900
C	3.15507400	-0.11865500	2.55765600	-2.30118200	-1.02288800	-2.15379800
C	3.75177400	-0.44052500	1.33547500	-3.30591700	-0.87462300	-1.19389100
N	3.65699500	0.21049100	0.09884200	-3.56876700	0.20214100	-0.33309700

H	-3.18787400	4.53387100	1.36869300	3.37092900	4.79903000	0.43564700
H	-4.56088000	2.51635700	0.88270700	4.63051400	2.63834900	0.55178200
H	-1.05410800	0.47545800	-0.51048700	0.98844400	0.44678200	-0.01478000
H	-0.76031500	4.53254400	0.89740900	0.95703000	4.82281500	0.18671700
H	1.05425300	0.47785400	0.50748200	-0.98815700	0.44658900	0.01436300
H	4.56117600	2.51255700	-0.89436500	-4.63059800	2.63743000	-0.55229600
H	3.18810300	4.52766200	-1.39004200	-3.37133000	4.79859200	-0.43624400
H	0.76046700	4.52834000	-0.91930800	-0.95739900	4.82267400	-0.18757900
H	-2.49613700	0.72421900	-2.65945700	1.55750300	-0.24884700	2.31332800
H	-2.98278100	-0.72864200	-4.60831000	1.51665300	-2.33132800	3.65778900
H	-4.49511000	-2.67898100	-4.39813100	3.21387300	-4.10303200	3.31453500
H	-5.57231200	-3.20799700	-2.22334800	5.01208700	-3.81210600	1.62507800
H	-6.42696300	-3.24221300	0.41862700	6.70153900	-2.88931700	-0.37014900
H	-6.82615700	-2.77585300	2.82540600	7.83543900	-1.57509900	-2.14685300
H	-5.70701800	-0.86576800	3.93660200	6.95310100	0.63537800	-2.83144500
H	-4.18286400	0.62914600	2.67516100	4.93308700	1.59074700	-1.75360800
H	4.18169100	0.61480000	-2.67883700	-4.93255000	1.59126500	1.75277600
H	5.70490100	-0.88718000	-3.93299400	-6.95308300	0.63683400	2.83070900
H	6.82411800	-2.79157000	-2.81217800	-7.83594300	-1.57358300	2.14663300
H	6.42577500	-3.24514900	-0.40279700	-6.70211000	-2.88877100	0.37066300
H	5.57288600	-3.19630100	2.23950000	-5.01236300	-3.81271900	-1.62401800
H	4.49671800	-2.65551500	4.41191500	-3.21380100	-4.10463600	-3.31295200
H	2.98464200	-0.70396200	4.61230100	-1.51618300	-2.33335900	-3.65650900
H	2.49741400	0.73860700	2.65595800	-1.55683300	-0.25045200	-2.31273500

Table S6. Optimized geometries (in Å) and energies (in hartree) of *p*-CBP in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1495.85102			Energy = -1495.751071		
C	-1.46852600	-1.14181500	0.37728900	1.48795000	-1.22826200	-0.03758600
C	-2.86011600	-1.14371400	0.38712200	2.85507600	-1.22268200	-0.03579000
C	-3.56984900	0.00012300	-0.00057600	3.58726200	-0.00001700	-0.00008200
C	-2.86006200	1.14388700	-0.38836600	2.85507300	1.22264800	0.03558200
C	-1.46847500	1.14188100	-0.37865700	1.48794700	1.22822800	0.03727100
C	-0.74138200	0.00001600	-0.00068400	0.70124400	-0.00001700	-0.00019300
C	2.86006200	-1.14389000	-0.38836500	-2.85508100	-1.22268500	0.03561400
C	1.46847500	-1.14188300	-0.37865600	-1.48797100	-1.22826500	0.03730600
C	0.74138200	-0.00001800	-0.00068500	-0.70124700	-0.00001400	-0.00024900
C	1.46852600	1.14181400	0.37728500	-1.48796300	1.22824300	-0.03783800
C	2.86011700	1.14371400	0.38711600	-2.85507200	1.22267500	-0.03602400
C	3.56984900	-0.00012500	-0.00057900	-3.58728400	0.00000000	-0.00015000

C	-6.48234900	2.77448700	2.01326100	6.49460100	2.34553900	-2.49975100
C	-7.83240000	2.46323200	1.77738600	7.84324500	2.09062400	-2.20131400
C	-8.17882100	1.37258700	0.98516500	8.18883200	1.16709400	-1.21693900
C	-7.16513000	0.59180900	0.41775100	7.17435700	0.50800200	-0.51680000
C	-5.80809700	0.92925200	0.65342400	5.81784000	0.79472100	-0.81215600
C	-5.45393700	2.01447600	1.45988100	5.46493400	1.69904600	-1.81814000
C	-5.80852900	-0.92886100	-0.65357800	5.81775500	-0.79477900	0.81219200
C	-7.16541300	-0.59165000	-0.41667500	7.17430300	-0.50803000	0.51701000
C	-8.17949200	-1.37256500	-0.98320600	8.18870400	-1.16710700	1.21726800
C	-7.83362100	-2.46313000	-1.77576700	7.84301200	-2.09066100	2.20158500
C	-6.48373500	-2.77413800	-2.01291900	6.49433600	-2.34561000	2.49984800
C	-5.45494200	-2.01396300	-1.46048100	5.46474100	-1.69912900	1.81811600
N	-4.98810900	0.00028100	-0.00046300	4.99183200	-0.00002200	-0.00001800
C	6.48234900	-2.77448800	2.01325900	-6.49469200	-2.34613700	-2.49915900
C	7.83240100	-2.46323100	1.77738600	-7.84332500	-2.09113900	-2.20074700
C	8.17882100	-1.37258500	0.98516700	-8.18888100	-1.16736400	-1.21658600
C	7.16513000	-0.59180800	0.41775100	-7.17438100	-0.50811700	-0.51663600
C	5.80809700	-0.92925300	0.65342100	-5.81787600	-0.79491100	-0.81197000
C	5.45393700	-2.01447800	1.45987700	-5.46499900	-1.69947800	-1.81774000
C	5.80852900	0.92886100	-0.65357900	-5.81772500	0.79497700	0.81199700
C	7.16541300	0.59165100	-0.41667400	-7.17428400	0.50817100	0.51693000
C	8.17949200	1.37256800	-0.98320300	-8.18865200	1.16742400	1.21706600
C	7.83362000	2.46313400	-1.77576400	-7.84290900	2.09122000	2.20114200
C	6.48373400	2.77414100	-2.01291700	-6.49421900	2.34623100	2.49928800
C	5.45494100	2.01396400	-1.46048100	-5.46465500	1.69956500	1.81767900
N	4.98810900	-0.00028300	-0.00046700	-4.99183700	0.00001600	-0.00004800
H	-0.93739400	-2.02953800	0.70847900	0.98318400	-2.18428200	-0.10525900
H	-3.40379600	-2.02356700	0.71647200	3.39940300	-2.15948000	-0.10515500
H	-3.40373000	2.02378500	-0.71764000	3.39939400	2.15944500	0.10500400
H	-0.93729700	2.02957200	-0.70985700	0.98317500	2.18424600	0.10492700
H	3.40373000	-2.02378900	-0.71763700	-3.39941300	-2.15947100	0.10512500
H	0.93729700	-2.02957500	-0.70985300	-0.98319500	-2.18427500	0.10504600
H	0.93739500	2.02953800	0.70847300	-0.98318200	2.18424100	-0.10571800
H	3.40379700	2.02356700	0.71646300	-3.39940600	2.15946100	-0.10554200
H	-6.23126600	3.62392700	2.64275100	6.24468300	3.05571200	-3.28313500
H	-8.61046000	3.07719600	2.22193500	8.62244000	2.61092900	-2.75085800
H	-9.22328200	1.12623100	0.81244700	9.23288700	0.95556800	-1.00153600
H	-4.41447000	2.25565300	1.65596000	4.42728100	1.88508900	-2.07152900
H	-9.22383800	-1.12638900	-0.80953200	9.23278100	-0.95555600	1.00199800
H	-8.61198900	-3.07719700	-2.21963300	8.62214800	-2.61095800	2.75122000
H	-6.23309500	-3.62348800	-2.64270800	6.24433500	-3.05579700	3.28319200
H	-4.41562700	-2.25491600	-1.65759700	4.42705900	-1.88519100	2.07137600

H	6.23126700	-3.62392900	2.64274800	-6.24479800	-3.05650500	-3.28237300
H	8.61046000	-3.07719400	2.22193700	-8.62253900	-2.61157100	-2.75014400
H	9.22328200	-1.12622700	0.81245100	-9.23292800	-0.95577700	-1.00120400
H	4.41447000	-2.25565700	1.65595400	-4.42735100	-1.88559100	-2.07110600
H	9.22383700	1.12639300	-0.80952700	-9.23273900	0.95582900	1.00188800
H	8.61198800	3.07720200	-2.21962800	-8.62201800	2.61165800	2.75068200
H	6.23309400	3.62349100	-2.64270500	-6.24417800	3.05661100	3.28244400
H	4.41562600	2.25491500	-1.65759800	-4.42695800	1.88568300	2.07084100

Table S7. Optimized geometries (in Å) and energies (in hartree) of *m*-CzCF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1612.5946			Energy = -1612.362686		
C	-1.17614700	2.95202100	0.08766000	1.17687400	2.94950800	-0.07327300
C	-2.53514600	3.22872900	0.18549200	2.51954100	3.21267400	-0.14577100
C	-3.44847300	2.17340300	0.26185000	3.44721000	2.14314900	-0.20046100
C	-3.00522100	0.84269400	0.21814800	2.98168900	0.78144100	-0.16502300
C	-1.63807600	0.55661100	0.11000800	1.64146700	0.48682800	-0.09202300
C	-0.73223300	1.61542400	0.05595400	0.69202700	1.56645000	-0.04931700
C	0.73233800	1.61545100	-0.05623200	-0.69199400	1.56643500	0.04948600
C	1.17622500	2.95205800	-0.08769200	-1.17687400	2.94951900	0.07323000
C	0.00003100	3.92329400	0.00004400	0.00000800	3.92461200	0.00007500
C	1.63819500	0.55665500	-0.11040500	-1.64142300	0.48680300	0.09225400
C	3.00535300	0.84277300	-0.21835500	-2.98165100	0.78139900	0.16496800
C	3.44858000	2.17349500	-0.26184400	-3.44722000	2.14313700	0.20007200
C	2.53522900	3.22879400	-0.18542400	-2.51955500	3.21267100	0.14541300
C	0.09429200	4.81037700	1.26228800	-0.07773300	4.81316200	-1.26210700
C	3.95827100	-1.25270700	-1.22560700	-3.93816300	-1.32906900	1.14689000
C	3.10315900	-1.47445900	-2.30874300	-3.02256800	-1.63857800	2.15641100
C	3.34978100	-2.58556700	-3.11233500	-3.27450500	-2.76379400	2.93891700
C	4.42292700	-3.45519500	-2.85181700	-4.40946300	-3.56460000	2.72814000
C	5.27833700	-3.22209500	-1.77899800	-5.32545100	-3.24389700	1.72990200
C	5.05359700	-2.11255700	-0.95553700	-5.09705100	-2.11754500	0.93235500
C	5.73446000	-1.57400000	0.20346200	-5.83522000	-1.49739500	-0.14890600
C	5.02726300	-0.40686400	0.58997900	-5.09808600	-0.35345900	-0.54643000
N	3.94952800	-0.21780900	-0.28295600	-3.94805100	-0.25178600	0.24730200
C	6.85403700	-1.97712500	0.94086500	-7.02443100	-1.81755600	-0.81165900
C	7.24662500	-1.22546500	2.04451500	-7.45779100	-1.00624100	-1.85753300
C	6.52610600	-0.07884400	2.42108100	-6.70530500	0.11213100	-2.25307400
C	5.40886100	0.34495400	1.70461500	-5.51465800	0.45006100	-1.61230200
C	-5.02713400	-0.40698500	-0.59016900	5.09811700	-0.35345700	0.54639300

C	-5.40864600	0.34467900	-1.70494600	5.51472900	0.45008700	1.61223400
C	-6.52607700	-0.07897600	-2.42119800	6.70536900	0.11213900	2.25300600
C	-7.24684500	-1.22534000	-2.04432000	7.45781800	-1.00626700	1.85749200
C	-6.85432900	-1.97687300	-0.94056400	7.02442500	-1.81760000	0.81164700
C	-5.73457800	-1.57388100	-0.20335100	5.83521400	-1.49742800	0.14889300
C	-5.05374800	-2.11235900	0.95569400	5.09702000	-2.11758600	-0.93234400
C	-3.95821100	-1.25269400	1.22551300	3.93814500	-1.32908500	-1.14688000
N	-3.94933500	-0.21796000	0.28268900	3.94808000	-0.25177400	-0.24733200
C	-5.27863200	-3.22171700	1.77936100	5.32537200	-3.24396500	-1.72986900
C	-4.42315500	-3.45482700	2.85212200	4.40936400	-3.56466100	-2.72809100
C	-3.34982300	-2.58535700	3.11241100	3.27442600	-2.76382900	-2.93887300
C	-3.10306700	-1.47442100	2.30862600	3.02252700	-1.63859300	-2.15638300
C	-0.09426000	4.81055200	-1.26207200	0.07776800	4.81281900	1.26248600
H	-2.89694900	4.25350800	0.21753600	2.88982500	4.23485600	-0.17202900
H	-4.51033000	2.37205900	0.36616300	4.50678500	2.33405400	-0.32198800
H	-1.30815500	-0.47664900	0.05895600	1.30986000	-0.54475900	-0.03962100
H	1.30828100	-0.47661900	-0.05957300	-1.30978100	-0.54478400	0.04007400
H	4.51045100	2.37217500	-0.36601200	-4.50682000	2.33403700	0.32137900
H	2.89702300	4.25358200	-0.21729400	-2.88986500	4.23484900	0.17145800
H	-0.78768500	5.45544600	1.34801800	0.80636100	5.45755300	-1.33687700
H	0.97883800	5.45596600	1.21615900	-0.96419500	5.45777300	-1.22780200
H	0.16201200	4.20120600	2.16918300	-0.13359600	4.20399500	-2.16978100
H	2.27782200	-0.80311100	-2.52172900	-2.14741500	-1.02233400	2.32988000
H	2.69745500	-2.77989500	-3.95941300	-2.57475000	-3.02445100	3.72825600
H	4.58615900	-4.31398800	-3.49663700	-4.57376900	-4.43833000	3.35225600
H	6.11328100	-3.89023900	-1.58413300	-6.20972700	-3.85657200	1.57483600
H	7.40625200	-2.86905700	0.65629500	-7.59888500	-2.69215800	-0.51778400
H	8.11453000	-1.52814200	2.62343700	-8.38024800	-1.24456800	-2.37930400
H	6.84299900	0.49007400	3.29104900	-7.05127500	0.72410700	-3.08160900
H	4.85246300	1.22603900	2.00699900	-4.92861300	1.30280600	-1.93758800
H	-4.85206400	1.22556500	-2.00756400	4.92871700	1.30286700	1.93748600
H	-6.84293200	0.48984900	-3.29124000	7.05136900	0.72412800	3.08151900
H	-8.11489000	-1.52791800	-2.62308500	8.38027000	-1.24461000	2.37926400
H	-7.40673500	-2.86861500	-0.65576800	7.59885800	-2.69222200	0.51779000
H	-6.11371600	-3.88973900	1.58467600	6.20962800	-3.85666700	-1.57480200
H	-4.58648500	-4.31349200	3.49708700	4.57364300	-4.43840700	-3.35219300
H	-2.69747200	-2.77966700	3.95947300	2.57466200	-3.02448100	-3.72820700
H	-2.27761300	-0.80316700	2.52145500	2.14739700	-1.02231800	-2.32985700
H	-0.97882000	5.45611900	-1.21586300	0.96424500	5.45742000	1.22834800
H	-0.16197100	4.20151300	-2.16905800	0.13362500	4.20341500	2.17000300
H	0.78770300	5.45565100	-1.34772600	-0.80631600	5.45720200	1.33743100

Table S8. Optimized geometries (in Å) and energies (in hartree) of *p*-CzCF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1612.5931			Energy = -1612.369185		
C	-1.18004700	0.01678200	0.26024100	1.18169300	0.30566000	0.02933400
C	-2.53757100	0.02366300	0.55021200	2.51653100	0.58026600	0.04962200
C	-3.46330200	0.04083100	-0.50632600	3.46106300	-0.50175200	0.04829200
C	-3.01672300	0.04323700	-1.83681100	2.99447300	-1.85170100	0.03888100
C	-1.65307900	0.01775400	-2.12671600	1.65565600	-2.14598400	0.02860700
C	-0.73300500	0.00899100	-1.07633500	0.69392400	-1.06760900	0.01529900
C	0.73300100	-0.00904400	-1.07634100	-0.69385600	-1.06767300	-0.01551100
C	1.18005500	-0.01682200	0.26023100	-1.18173100	0.30555500	-0.03035700
C	0.00000800	-0.00001700	1.23222900	-0.00004900	1.27920300	-0.00101600
C	1.65306600	-0.01781700	-2.12673000	-1.65552000	-2.14612700	-0.02807800
C	3.01671300	-0.04329100	-1.83683500	-2.99435400	-1.85194000	-0.03824100
C	3.46330300	-0.04086800	-0.50635400	-3.46105800	-0.50202500	-0.04824700
C	2.53758100	-0.02369500	0.55019200	-2.51658700	0.58005800	-0.05049800
C	-0.01569600	-1.26575900	2.11860300	0.03056500	2.16493000	-1.26634700
C	5.79694900	0.86610100	-0.70355300	-5.80187300	-0.80467400	0.79068100
C	5.60631400	1.99670600	-1.50286500	-5.62550700	-1.70062500	1.84925300
C	6.72569300	2.76380500	-1.81876000	-6.75728900	-2.09499100	2.56067900
C	8.00533700	2.42154200	-1.34872300	-8.03290300	-1.60246200	2.23892300
C	8.18662600	1.30233000	-0.54156900	-8.19854000	-0.68951900	1.19957800
C	7.07860900	0.51431600	-0.20842700	-7.07919400	-0.28056800	0.46883700
C	6.90427400	-0.67336600	0.60143600	-6.88774900	0.65231400	-0.62369500
C	5.52321400	-0.99491400	0.56785600	-5.50227300	0.65476600	-0.92436200
N	4.85608100	-0.05528600	-0.22753300	-4.84177400	-0.23382200	-0.06061900
C	7.78365500	-1.48389500	1.32887700	-7.75911000	1.44928400	-1.37178100
C	7.28369100	-2.59563900	2.00060000	-7.24600300	2.22678400	-2.40783400
C	5.91442700	-2.90789600	1.94484100	-5.87411300	2.20059300	-2.70862500
C	5.01745900	-2.11783300	1.22889200	-4.98534700	1.41244200	-1.97956600
C	-5.52319900	0.99491600	0.56787200	5.50207700	0.65573100	0.92404700
C	-5.01742500	2.11782800	1.22890400	4.98490300	1.41431300	1.97847400
C	-5.91438600	2.90792700	1.94482500	5.87351300	2.20302900	2.70711200
C	-7.28366000	2.59571000	2.00056100	7.24548400	2.22891500	2.40665800
C	-7.78364100	1.48397200	1.32884100	7.75883000	1.45054600	1.37137600
C	-6.90426900	0.67341000	0.60142700	6.88763200	0.65298600	0.62372700
C	-7.07862200	-0.51427800	-0.20842400	7.07932900	-0.28084000	-0.46795400
C	-5.79696200	-0.86610600	-0.70351900	5.80207700	-0.80520500	-0.78963900
N	-4.85607600	0.05525600	-0.22748800	4.84176300	-0.23347100	0.06078800
C	-8.18665500	-1.30226500	-0.54157600	8.19883900	-0.69050300	-1.19804700
C	-8.00538200	-2.42149300	-1.34871100	8.03342600	-1.60443700	-2.23655600

C	-6.72573900	-2.76379900	-1.81871900	6.75787700	-2.09726300	-2.55813900
C	-5.60634400	-1.99672900	-1.50281200	5.62593600	-1.70219000	-1.84736400
C	0.01571900	1.26573000	2.11859800	-0.03071600	2.16651300	1.26316400
H	-2.90021300	0.00433700	1.57399200	2.88687700	1.60115800	0.02885700
H	-3.74757100	0.07678200	-2.63850500	3.72776600	-2.65147900	0.07763000
H	-1.32063700	0.01923500	-3.16144400	1.32089300	-3.17883100	0.04655700
H	1.32061600	-0.01931100	-3.16145500	-1.32068700	-3.17896000	-0.04557900
H	3.74755600	-0.07684300	-2.63853400	-3.72758700	-2.65179400	-0.07649600
H	2.90023100	-0.00435900	1.57396900	-2.88698900	1.60094100	-0.03028700
H	-0.90132200	-1.27500600	2.76408900	0.91888600	2.80760400	-1.26821400
H	0.86983200	-1.29587800	2.76378600	-0.85449100	2.81103200	-1.30754100
H	-0.02742400	-2.17484600	1.50891500	0.05055500	1.55337600	-2.17401200
H	4.62040800	2.27287400	-1.86180200	-4.64186200	-2.06940400	2.11806100
H	6.60266600	3.64682700	-2.44008400	-6.64572500	-2.79321100	3.38567200
H	8.85796800	3.03966700	-1.61511800	-8.89522500	-1.92960000	2.81275900
H	9.17512600	1.04466200	-0.17013800	-9.18331100	-0.29418700	0.96467600
H	8.84444400	-1.24940300	1.36401700	-8.82377500	1.45508700	-1.15334600
H	7.95630400	-3.23118800	2.56952000	-7.91273800	2.85131900	-2.99546200
H	5.54442800	-3.78574900	2.46775200	-5.49515500	2.80065000	-3.53138600
H	3.96363300	-2.37174600	1.18224900	-3.93141600	1.38160900	-2.23251000
H	-3.96359100	2.37171100	1.18227900	3.93089700	1.38376500	2.23114400
H	-5.54437100	3.78577600	2.46773200	5.49436200	2.80380100	3.52926200
H	-7.95626500	3.23128300	2.56946100	7.91209100	2.85391100	2.99394100
H	-8.84443700	1.24950900	1.36396300	8.82355300	1.45612500	1.15321600
H	-9.17515500	-1.04456400	-0.17016700	9.18356900	-0.29499500	-0.96327000
H	-8.85802600	-3.03959500	-1.61511600	8.89588100	-1.93215400	-2.80986200
H	-6.60272500	-3.64683200	-2.44003000	6.64649900	-2.79628200	-3.38248000
H	-4.62043900	-2.27292900	-1.86172700	4.64233300	-2.07121800	-2.11601400
H	-0.86980100	1.29585000	2.76379000	0.85428600	2.81274000	1.30354500
H	0.02743900	2.17481200	1.50890400	-0.05067500	1.55612000	2.17161200
H	0.90135200	1.27498300	2.76407300	-0.91906400	2.80915200	1.26422700

Table S9. Optimized geometries (in Å) and energies (in hartree) of *m*-CzSiF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1864.0077			Energy = -1863.775968		
C	-3.52309500	2.04387900	-0.31607900	3.51567800	2.01765700	0.24007800
C	-2.92470000	0.77847200	-0.25849100	2.90350000	0.70980000	0.19439100
C	-1.53524900	0.66361700	-0.12663100	1.54215500	0.57545300	0.10452500
C	-0.74165500	1.81246400	-0.06707800	0.69820600	1.73673300	0.05637200
C	-1.34071700	3.09730400	-0.11761100	1.32782400	3.07784700	0.09681500

C	-2.72917100	3.18952600	-0.23516500	2.71094100	3.16056400	0.18648700
C	1.34070100	3.09738900	0.11755400	-1.32814900	3.07771000	-0.09718400
C	0.74171800	1.81250900	0.06712000	-0.69843800	1.73666500	-0.05617900
C	1.53537400	0.66371500	0.12679900	-1.54229200	0.57530600	-0.10407700
C	2.92482000	0.77865300	0.25870300	-2.90361000	0.70951300	-0.19456200
C	3.52312900	2.04410800	0.31622400	-3.51585200	2.01730000	-0.24113200
C	2.72914400	3.18970300	0.23515900	-2.71122800	3.16028900	-0.18758700
Si	-0.00003700	4.41816800	-0.00011700	-0.00024400	4.40329600	-0.00001100
C	0.13680000	5.49985500	-1.54428100	-0.11446700	5.51035600	1.53303700
C	-0.13696600	5.50015200	1.54382900	0.11391900	5.51104500	-1.53255000
C	6.42554100	-0.52711800	-2.24907400	-6.57381900	-0.37034200	2.15513600
C	6.98151500	-1.75974200	-1.86593500	-7.18923700	-1.56545300	1.74741200
C	6.44847900	-2.47438800	-0.79713500	-6.64755800	-2.32427500	0.71241800
C	5.35440900	-1.94714600	-0.10131700	-5.48855500	-1.87393700	0.07252800
C	4.81464800	-0.69528600	-0.49249000	-4.89139100	-0.65486000	0.48174900
C	5.33690600	0.02054200	-1.57355400	-5.41509500	0.09751500	1.53774600
C	3.56516200	-1.43591900	1.25406200	-3.59744900	-1.49515200	-1.18670500
C	4.55979900	-2.41770200	1.01398200	-4.66456500	-2.40833800	-0.99266200
C	4.61224000	-3.55883100	1.82295400	-4.74977700	-3.55283500	-1.79235700
C	3.68808000	-3.70312600	2.85348000	-3.78470200	-3.76841000	-2.77258800
C	2.71782600	-2.71340000	3.08655500	-2.74321100	-2.84509600	-2.96369200
C	2.64348100	-1.56826700	2.29636200	-2.63435800	-1.69904800	-2.17849200
N	3.72624600	-0.39104600	0.33479700	-3.74468400	-0.42524700	-0.28981400
C	-2.71733400	-2.71374000	-3.08607200	2.74477600	-2.84344300	2.96538600
C	-3.68772400	-3.70337200	-2.85318200	3.78623500	-3.76677700	2.77420600
C	-4.61209900	-3.55897000	-1.82286100	4.75079200	-3.55162100	1.79337300
C	-4.55976600	-2.41780400	-1.01393800	4.66508800	-2.40753000	0.99314900
C	-3.56494400	-1.43614600	-1.25379100	3.59800400	-1.49432500	1.18728300
C	-2.64304000	-1.56860300	-2.29587400	2.63543700	-1.69779500	2.17966900
C	-4.81467600	-0.69538200	0.49252100	4.89103200	-0.65476800	-0.48225000
C	-5.35455300	-1.94715100	0.10119900	5.48849600	-1.87359600	-0.07272400
C	-6.44893700	-2.47416900	0.79669000	6.64721100	-2.32415900	-0.71297800
C	-6.98210900	-1.75943700	1.86536900	7.18830700	-1.56580900	-1.74862200
C	-6.42598400	-0.52694100	2.24869100	6.57259500	-0.37094500	-2.15662500
C	-5.33706700	0.02052500	1.57346500	5.41414700	0.09712800	-1.53888200
N	-3.72604300	-0.39130200	-0.33450400	3.74470600	-0.42485100	0.28978900
H	-4.59903200	2.12048900	-0.43724900	4.59009100	2.09343800	0.36321000
H	-1.09866700	-0.32792800	-0.06068400	1.11003600	-0.41827700	0.04956400
H	-3.21300400	4.16306100	-0.28058600	3.19714400	4.13373800	0.22777400
H	1.09884200	-0.32785800	0.06095800	-1.11012000	-0.41836900	-0.04852600
H	4.59905600	2.12079600	0.43744200	-4.59021500	2.09295400	-0.36478300
H	3.21291700	4.16327000	0.28054400	-3.19748900	4.13340900	-0.22943500

H	1.02135200	6.14656500	-1.49608100	-1.00116400	6.15532900	1.48865100
H	-0.74035800	6.14973100	-1.64999300	0.76239900	6.16507400	1.61397700
H	0.21470700	4.88924200	-2.45004200	-0.17637200	4.91547600	2.45036800
H	0.73959900	6.15094500	1.64880300	-0.76264700	6.16624300	-1.61284200
H	-1.02220300	6.14595300	1.49602000	1.00094400	6.15556700	-1.48812400
H	-0.21369000	4.88970700	2.44980400	0.17523600	4.91662100	-2.45021500
H	6.84935500	0.01190500	-3.09214100	-7.00191700	0.19927700	2.97544200
H	7.83132900	-2.15839100	-2.41264700	-8.08949900	-1.90476100	2.25171600
H	6.87279500	-3.43251300	-0.50825800	-7.11525500	-3.25755300	0.40986200
H	4.90718300	0.96768600	-1.88241100	-4.93301100	1.00900500	1.87435400
H	5.36873400	-4.31988900	1.64984700	-5.56277900	-4.26059400	-1.65303200
H	3.71764600	-4.58535800	3.48653700	-3.83809900	-4.65502800	-3.39785100
H	2.01013600	-2.83936100	3.90146200	-2.00398000	-3.02505900	-3.73940100
H	1.89809300	-0.80421300	2.49057000	-1.83137500	-0.98802900	-2.33811900
H	-2.00947700	-2.83978400	-3.90082100	2.00596200	-3.02307200	3.74156800
H	-3.71722200	-4.58562600	-3.48621400	3.84002100	-4.65307700	3.39988500
H	-5.36871800	-4.31994300	-1.64992400	5.56377500	-4.25938900	1.65398900
H	-1.89755000	-0.80461500	-2.48994700	1.83249000	-0.98675200	2.33935500
H	-6.87335300	-3.43221500	0.50769900	7.11513400	-3.25725200	-0.41019900
H	-7.83215800	-2.15792100	2.41183600	8.08834000	-1.90529900	-2.25321200
H	-6.84991400	0.01214600	3.09165900	7.00024000	0.19830300	-2.97742600
H	-4.90722300	0.96756800	1.88246300	4.93182800	1.00841900	-1.87569000

Table S10. Optimized geometries (in Å) and energies (in hartree) of *p*-CzSiF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1864.006			Energy = -1863.782577		
C	-3.54221100	-0.07031900	-0.44978300	3.52977000	-0.43987200	0.00985000
C	-2.93834000	-0.34688500	-1.68339400	2.91517500	-1.73863400	0.00451600
C	-1.55029900	-0.38823400	-1.79692300	1.55633900	-1.87060500	0.00948800
C	-0.74197900	-0.13554900	-0.68223200	0.69911100	-0.70778100	0.00675700
C	-1.34720100	0.15617100	0.56766700	1.33606500	0.62412500	0.01943600
C	-2.73693000	0.17709500	0.67264300	2.71094500	0.71653200	0.02243800
C	1.34688100	0.13282200	0.57497400	-1.33598300	0.62432500	-0.01795300
C	0.74374000	-0.14653100	-0.67872300	-0.69905700	-0.70770600	-0.00923900
C	1.55328700	-0.40548000	-1.79124100	-1.55639800	-1.87047000	-0.01498100
C	2.94118300	-0.39820100	-1.66806800	-2.91517200	-1.73840000	-0.00955800
C	3.54269600	-0.11480900	-0.43503400	-3.52979200	-0.43956600	-0.01151600
C	2.73657800	0.15389000	0.68151200	-2.71082800	0.71683300	-0.02067800
Si	-0.00115200	0.44278800	1.85930500	0.00010800	1.94826000	0.00260600
C	0.01178500	2.19854200	2.55779700	-0.02152500	3.05076200	1.54280000

C	-0.01449500	-0.82308900	3.26233500	0.02220600	3.05484200	-1.53463900
C	6.26679900	-2.45217000	2.27482900	-6.25020300	1.99778600	-2.63834700
C	7.63228700	-2.16163100	2.11124600	-7.61500600	1.85706100	-2.33737100
C	8.04856500	-1.22496900	1.16966700	-8.03042500	1.01060100	-1.31186500
C	7.08933100	-0.56808300	0.39008000	-7.06916800	0.31356100	-0.57404800
C	5.71478900	-0.86311400	0.57843700	-5.69425900	0.48503200	-0.87383500
C	5.29141700	-1.81256500	1.51272400	-5.27291000	1.31226300	-1.91894000
C	5.83480900	0.68316200	-1.07949400	-5.81708700	-1.02033200	0.82429300
C	7.16580900	0.41936800	-0.66630200	-7.14765300	-0.64791400	0.50765100
C	8.22533600	1.09850600	-1.27922200	-8.21002900	-1.19440600	1.23338800
C	7.94895200	2.02565300	-2.27979600	-7.93656800	-2.09193600	2.26335100
C	6.62296200	2.28476800	-2.66735900	-6.61141300	-2.43260900	2.58096000
C	5.55001700	1.62271500	-2.07430800	-5.53489700	-1.89864300	1.87476500
N	4.95813200	-0.09932300	-0.31825500	-4.93237000	-0.32976800	-0.01987200
C	-6.29301200	3.13984200	1.09422300	6.24950600	1.98294200	2.65024300
C	-7.65488200	2.79329500	1.06924300	7.61442800	1.84354400	2.34913500
C	-8.06009900	1.55222900	0.58696600	8.03014900	1.00270800	1.31913900
C	-7.09328700	0.64730400	0.13358800	7.06908600	0.30992500	0.57703800
C	-5.72214900	1.00717900	0.18010100	5.69409900	0.47992400	0.87731400
C	-5.31033700	2.25776800	0.64965600	5.27240300	1.30155300	1.92667100
C	-5.82653700	-1.07646300	-0.71646000	5.81717100	-1.01557800	-0.82943600
C	-7.15970900	-0.68201900	-0.43659300	7.14773100	-0.64526800	-0.51020200
C	-8.21268400	-1.56002800	-0.71915100	8.21019100	-1.18756000	-1.23897500
C	-7.92762100	-2.80851700	-1.26420700	7.93680800	-2.07872600	-2.27446500
C	-6.59942900	-3.18873400	-1.52258400	6.61165400	-2.41707400	-2.59459800
C	-5.53309900	-2.33387000	-1.25170200	5.53503400	-1.88724000	-1.88545200
N	-4.95724500	-0.04529500	-0.33810600	4.93241800	-0.32997700	0.01863200
H	-3.56363400	-0.52084700	-2.55350100	3.55198900	-2.61695200	0.03957000
H	-1.10942200	-0.60626600	-2.76572800	1.11913900	-2.86471800	0.03288600
H	-3.22167000	0.37216900	1.62585100	3.19976700	1.68775300	0.00224200
H	1.11331100	-0.62885100	-2.75922400	-1.11926200	-2.86454700	-0.04084700
H	3.56792500	-0.62338400	-2.52546800	-3.55211400	-2.61652800	-0.04611900
H	3.22103000	0.38863200	1.62604900	-3.19949300	1.68804500	0.00258400
H	0.90984900	2.37531100	3.16199300	-0.90644700	3.69951000	1.55193400
H	-0.85826500	2.37360000	3.20221200	0.86175500	3.70104200	1.57613200
H	-0.00606900	2.94419200	1.75588600	-0.03461000	2.45180600	2.45952200
H	-0.00628900	-1.84693300	2.87366300	0.03292200	2.45823000	-2.45292200
H	-0.90763500	-0.70749500	3.88821300	0.90865400	3.70152200	-1.54309600
H	0.86064700	-0.70063400	3.91193900	-0.85957800	3.70727100	-1.56529500
H	5.96208600	-3.19375400	3.00842700	-5.94625100	2.64926700	-3.45305200
H	8.36755300	-2.67705200	2.72259300	-8.35203400	2.40596600	-2.91648600
H	9.10552800	-1.00890600	1.03690000	-9.08778900	0.88713700	-1.09290200

H	4.24002800	-2.05005500	1.63707300	-4.22331800	1.41084200	-2.17232500
H	9.25061500	0.90649700	-0.97352000	-9.23490200	-0.91603800	1.00235000
H	8.76319300	2.55760200	-2.76358100	-8.75360400	-2.52461900	2.83353200
H	6.42645100	3.01878000	-3.44422900	-6.41697100	-3.12070200	3.39903800
H	4.52873700	1.83529600	-2.37272700	-4.51436100	-2.14957800	2.14184500
H	-5.99673800	4.11764800	1.46444700	5.94531800	2.63008700	3.46831200
H	-8.39602400	3.50341800	1.42483400	8.35130500	2.38908600	2.93161100
H	-9.11442300	1.28954800	0.55743500	9.08758800	0.88031400	1.09992700
H	-4.26222400	2.53785100	0.66138900	4.22266400	1.39909500	2.17990900
H	-9.23957000	-1.27078500	-0.51093400	9.23505900	-0.91078100	-1.00600500
H	-8.73665300	-3.49766700	-1.48898400	8.75389800	-2.50808800	-2.84707800
H	-6.39583300	-4.17094900	-1.94054400	6.41731200	-3.09995300	-3.41706000
H	-4.51013400	-2.63797300	-1.44688100	4.51452000	-2.13588900	-2.15482400

Table S11. Optimized geometries (in Å) and energies (in hartree) of *m*-CzGeF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -3649.5081			Energy = -3649.276376		
C	3.52923800	1.76876200	0.31974400	3.52429900	1.74442200	0.24741400
C	2.91450000	0.51160100	0.26088500	2.89293600	0.44884800	0.19856900
C	1.52453200	0.41641900	0.12724000	1.53033700	0.33478000	0.10438700
C	0.74204800	1.57384100	0.06720500	0.69785400	1.50853600	0.05583800
C	1.36261800	2.84463700	0.11977500	1.35467300	2.83203900	0.09922400
C	2.74901600	2.92308000	0.23864300	2.73112300	2.90083500	0.19093700
C	-1.36255900	2.84463600	-0.11962900	-1.35522000	2.83174400	-0.09994400
C	-0.74200400	1.57383700	-0.06709300	-0.69817000	1.50837000	-0.05556000
C	-1.52446800	0.41641100	-0.12715100	-1.53042500	0.33443700	-0.10367200
C	-2.91445600	0.51154800	-0.26076600	-2.89297900	0.44818500	-0.19886000
C	-3.52917400	1.76873700	-0.31956300	-3.52452800	1.74363600	-0.24917500
C	-2.74896400	2.92305500	-0.23843400	-2.73160400	2.90022800	-0.19282600
Ge	0.00003100	4.22023800	-0.00004200	-0.00044500	4.20961100	-0.00009600
C	-0.14085600	5.35155300	1.58275700	-0.11732600	5.35859900	1.57651500
C	0.14081900	5.35099400	-1.58325800	0.11624400	5.36007100	-1.57561500
C	-6.38653600	-0.85154800	2.25543000	-6.54596500	-0.69499600	2.14822300
C	-6.92865500	-2.08913700	1.86831000	-7.14214800	-1.89902200	1.73803200
C	-6.39100500	-2.79194200	0.79396000	-6.58822700	-2.64709300	0.70172300
C	-5.30615800	-2.24791400	0.09663300	-5.43611700	-2.17741700	0.06323900
C	-4.78032100	-0.99146500	0.49221600	-4.85829100	-0.94992300	0.47533000
C	-5.30735100	-0.28719200	1.57852400	-5.39462100	-0.20764600	1.53216400
C	-3.52919000	-1.70692800	-1.26330800	-3.55082000	-1.76603100	-1.19436800
C	-4.51033900	-2.70254200	-1.02440600	-4.60362400	-2.69628300	-1.00295200

C	-4.55140800	-3.84002900	-1.83916200	-4.67048300	-3.84011400	-1.80541100
C	-3.62949400	-3.96718100	-2.87395500	-3.70176200	-4.03829700	-2.78565100
C	-2.67258200	-2.96412800	-3.10539700	-2.67449100	-3.09854300	-2.97379300
C	-2.60963500	-1.82229500	-2.30948000	-2.58389000	-1.95285100	-2.18580000
N	-3.69953000	-0.66932800	-0.33781200	-3.71520900	-0.70091000	-0.29508100
C	2.67286400	-2.96384000	3.10573000	2.67728900	-3.09546200	2.97678700
C	3.62966400	-3.96697900	2.87420100	3.70443100	-4.03532600	2.78848900
C	4.55145500	-3.83997100	1.83927900	4.67224000	-3.83793200	1.80718800
C	4.51040600	-2.70251700	1.02447500	4.60459600	-2.69477800	1.00383000
C	3.52935400	-1.70681500	1.26348100	3.55192900	-1.76441000	1.19544900
C	2.60991800	-1.82203400	2.30977000	2.58591100	-1.95043500	2.18791600
C	4.78019800	-0.99153100	-0.49228900	4.85777900	-0.94964900	-0.47616000
C	5.30607400	-2.24798100	-0.09671500	5.43605400	-2.17677400	-0.06359200
C	6.39082700	-2.79201200	-0.79418900	6.58760500	-2.64689900	-0.70275300
C	6.92830000	-2.08924100	-1.86865300	7.14053200	-1.89963100	-1.74017300
C	6.38613500	-0.85166700	-2.25574600	6.54392100	-0.69595600	-2.15077600
C	5.30704900	-0.28728700	-1.57869700	5.39312000	-0.20816700	-1.53405200
N	3.69959600	-0.66930500	0.33790700	3.71543000	-0.70004400	0.29512300
H	4.60594900	1.83226900	0.44128800	4.59901900	1.80643600	0.37378900
H	1.07788900	-0.57045500	0.06108100	1.08716600	-0.65353600	0.04637800
H	3.23912500	3.89317700	0.28398700	3.22481600	3.86993500	0.23200100
H	-1.07777400	-0.57043900	-0.06102300	-1.08710400	-0.65374800	-0.04461100
H	-4.60588400	1.83228600	-0.44109200	-4.59915800	1.80538200	-0.37642400
H	-3.23909700	3.89314000	-0.28380700	-3.22544700	3.86921100	-0.23483100
H	-1.02582500	5.99185400	1.50640500	-1.00654500	5.99468400	1.50967000
H	0.74094100	5.99593700	1.66108300	0.76306200	6.00794700	1.63150400
H	-0.21898600	4.75026400	2.49197600	-0.17606100	4.76728700	2.49375200
H	-0.74121100	5.99501200	-1.66198800	-0.76390100	6.00983000	-1.62960700
H	1.02554200	5.99165000	-1.50706700	1.00572400	5.99575100	-1.50840500
H	0.21928100	4.74934100	-2.49220900	0.17444100	4.76969800	-2.49348900
H	-6.81389100	-0.32190600	3.10265500	-6.98354100	-0.13366300	2.96925600
H	-7.77139600	-2.50089900	2.41625800	-8.03714700	-2.25348400	2.24129100
H	-6.80476600	-3.75372300	0.50193400	-7.04135200	-3.58685000	0.39702600
H	-4.88816600	0.66387000	1.88991900	-4.92728200	0.71111100	1.86985600
H	-5.29740200	-4.61163700	-1.66718000	-5.47225100	-4.56097500	-1.66813000
H	-3.65029900	-4.84640900	-3.51152900	-3.74100100	-4.92417800	-3.41301100
H	-1.96632600	-3.07704800	-3.92346200	-1.93189300	-3.26532400	-3.74924100
H	-1.87448800	-1.04790900	-2.50195000	-1.79162200	-1.22924800	-2.34251300
H	1.96670800	-3.07667900	3.92389200	1.93541200	-3.26163000	3.75305800
H	3.65045900	-4.84619400	3.51179600	3.74428500	-4.92067700	3.41655800
H	5.29735900	-4.61166000	1.66726500	5.47391300	-4.55887400	1.66978000
H	1.87487200	-1.04755600	2.50225900	1.79374800	-1.22673700	2.34472700

H	6.80463900	-3.75378900	-0.50222000	7.04106600	-3.58638200	-0.39771400
H	7.77097700	-2.50101400	-2.41669300	8.03508800	-2.25444900	-2.24396900
H	6.81337900	-0.32206400	-3.10305100	6.98073100	-0.13524900	-2.97264500
H	4.88779800	0.66377000	-1.89002400	4.92544000	0.71031700	-1.87201900

Table S12. Optimized geometries (in Å) and energies (in hartree) of *p*-CzGeF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -3649.5068			Energy = -3649.284052		
C	3.54837700	-0.57156600	-0.01224700	3.53893500	-0.56195700	-0.00206700
C	2.92983700	-1.82837900	-0.03053000	2.90611300	-1.84830200	-0.00141300
C	1.54069700	-1.92903700	-0.01822900	1.54488700	-1.96083700	0.00565900
C	0.74300700	-0.77769700	-0.00741200	0.69927900	-0.78597000	0.00357300
C	1.36839300	0.49228200	0.00188500	1.36188000	0.52761200	0.00821500
C	2.75605000	0.58552000	0.00908100	2.73091800	0.60753500	0.00529200
C	-1.36836900	0.49241800	0.00456200	-1.36189900	0.52760400	-0.00827300
C	-0.74312500	-0.77763100	-0.00490800	-0.69928100	-0.78597300	-0.00372900
C	-1.54091500	-1.92894300	-0.01106900	-1.54487400	-1.96085200	-0.00590200
C	-2.93004100	-1.82834600	0.00299300	-2.90610200	-1.84833900	0.00118900
C	-3.54843700	-0.57133200	0.00365400	-3.53894000	-0.56200500	0.00195200
C	-2.75602900	0.58585900	-0.00090800	-2.73093600	0.60750200	-0.00533000
Ge	0.00009600	1.87041200	0.01290200	-0.00001200	1.90436500	0.00000100
C	-0.00111100	2.98710700	1.61088900	-0.01067900	3.05287200	1.58054800
C	0.00143900	3.00822500	-1.57010700	0.01070400	3.05282800	-1.58057900
C	-6.28090400	1.57487500	2.85484300	-6.26151800	1.87401800	-2.61726300
C	-7.64645300	1.46377300	2.54094600	-7.62702300	1.72039900	-2.32572200
C	-8.06009500	0.73178700	1.43179700	-8.04220200	0.86242600	-1.30966400
C	-7.09822500	0.11176800	0.62561800	-7.08013700	0.16662400	-0.57179300
C	-5.72387900	0.24591300	0.94917000	-5.70487200	0.35081600	-0.86215600
C	-5.30297500	0.96837400	2.06934000	-5.28322600	1.18991300	-1.89788700
C	-5.83897500	-1.05782300	-0.90622900	-5.82576200	-1.16873900	0.82325500
C	-7.17148400	-0.71785500	-0.55894800	-7.15741600	-0.80418200	0.50166900
C	-8.22982000	-1.18229200	-1.34856000	-8.21969200	-1.36485100	1.21663700
C	-7.95079600	-1.96480800	-2.46523600	-7.94524100	-2.26839600	2.24109200
C	-6.62341300	-2.28050800	-2.80289300	-6.61929400	-2.60101500	2.56402800
C	-5.55160800	-1.83209500	-2.03385400	-5.54290200	-2.05314200	1.86839900
N	-4.96414700	-0.46867400	0.01477600	-4.94159500	-0.46487700	-0.01033500
C	6.28119500	1.62320000	-2.82587900	6.26141400	1.87383800	2.61748100
C	7.64666900	1.50712900	-2.51349000	7.62693400	1.72019500	2.32602600
C	8.06017500	0.75627700	-1.41698000	8.04215200	0.86228300	1.30993200
C	7.09820600	0.12229100	-0.62185700	7.08011200	0.16657500	0.57194200

C	5.72391900	0.26172200	-0.94337300	5.70483000	0.35078900	0.86221900
C	5.30318100	1.00305400	-2.05119800	5.28314700	1.18982400	1.89798400
C	5.83880700	-1.07341800	0.88961000	5.82579800	-1.16864100	-0.82330100
C	7.17134800	-0.72750100	0.54832800	7.15743600	-0.80414100	-0.50160100
C	8.22963700	-1.20517000	1.33004700	8.21974900	-1.36476700	-1.21654900
C	7.95058300	-2.00638600	2.43338400	7.94534600	-2.26821400	-2.24110300
C	6.62318700	-2.32770500	2.76559700	6.61941100	-2.60077300	-2.56415600
C	5.55142100	-1.86650200	2.00409700	5.54298600	-2.05293900	-1.86854800
N	4.96407200	-0.46886600	-0.02148100	4.94159000	-0.46481400	0.01028000
H	3.54318100	-2.72332900	-0.06703000	3.52866700	-2.73685300	0.03415900
H	1.08933300	-2.91704700	-0.03348100	1.09653200	-2.94944700	0.03261500
H	3.24590200	1.55505100	0.03981800	3.22487500	1.57553200	-0.02010900
H	-1.08962100	-2.91710100	-0.01062800	-1.09650200	-2.94945300	-0.03294000
H	-3.54351500	-2.72366500	0.02600500	-3.52863900	-2.73689900	-0.03445400
H	-3.24583400	1.55576600	-0.01726400	-3.22491600	1.57548600	0.02013700
H	-0.88904300	3.62772700	1.61785400	-0.89799600	3.69494200	1.56882400
H	0.88464300	3.63069300	1.61613100	0.87589700	3.69612400	1.58125900
H	0.00181700	2.37791800	2.51817700	-0.01804100	2.46085400	2.49918000
H	-0.00118100	2.41083200	-2.48521200	0.01790200	2.46075100	-2.49917700
H	-0.88444900	3.65164100	-1.56721900	-0.87576400	3.69622600	-1.58127100
H	0.88929100	3.64899400	-1.56857500	0.89813700	3.69473900	-1.56896300
H	-5.97790600	2.14291900	3.73032800	-5.95782200	2.53464600	-3.42467300
H	-8.38383200	1.95026000	3.17308900	-8.36472400	2.26837200	-2.90486600
H	-9.11704800	0.63819100	1.19600900	-9.09991100	0.72921200	-1.09820000
H	-4.25142800	1.05069600	2.32374600	-4.23278000	1.29880500	-2.14350100
H	-9.25613200	-0.93006300	-1.09447700	-9.24536500	-1.09280600	0.98162800
H	-8.76394400	-2.33204500	-3.08485900	-8.76219700	-2.71216400	2.80280900
H	-6.42502900	-2.88490600	-3.68395500	-6.42424100	-3.29394900	3.37786700
H	-4.52922800	-2.07141500	-2.30710300	-4.52203900	-2.29795200	2.13981500
H	5.97833000	2.20603600	-3.69163400	5.95768100	2.53441500	3.42491900
H	8.38409200	2.00463100	-3.13695000	8.36461300	2.26810100	2.90526200
H	9.11707500	0.65886400	-1.18251300	9.09986900	0.72904600	1.09852500
H	4.25171200	1.08931500	-2.30456600	4.23269000	1.29873700	2.14354300
H	9.25595700	-0.94863400	1.08034700	9.24541200	-1.09276600	-0.98144400
H	8.76371000	-2.38398100	3.04677300	8.76232700	-2.71195100	-2.80280800
H	6.42472400	-2.94680500	3.63637300	6.42439600	-3.29362600	-3.37807300
H	4.52905500	-2.11044000	2.27328900	4.52213500	-2.29769600	-2.14005800

Table S13. Optimized geometries (in Å) and energies (in hartree) of *m*-CzNF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1589.3238			Energy = -1589.101526		
C	1.12350300	2.94448700	0.06701900	1.14702800	2.93115200	-0.09600800
C	2.47375900	3.30136000	0.13209600	2.48209300	3.29996700	-0.20691500
C	3.41666700	2.28076400	0.20088500	3.45210800	2.27712700	-0.25732200
C	3.03309700	0.92429700	0.17778300	3.04733700	0.92200700	-0.21047000
C	1.68519400	0.57168000	0.09461900	1.69481000	0.54221800	-0.11063400
C	0.72084800	1.58215800	0.04790700	0.71064600	1.55339500	-0.05379000
C	-0.72388100	1.58092800	-0.04188700	-0.70509300	1.56217200	0.06338100
C	-1.12827300	2.94256300	-0.07002000	-1.11911100	2.93058300	0.08196700
N	-0.00398600	3.75396500	0.01352800	0.02254200	3.72632800	0.00004000
C	-1.68686400	0.56885600	-0.08312200	-1.69941800	0.55905200	0.14256800
C	-3.03441300	0.91908500	-0.18048900	-3.06546100	0.96402900	0.22910800
C	-3.41872700	2.27480400	-0.22783600	-3.44215600	2.30404000	0.23648600
C	-2.47743500	3.29715700	-0.16474700	-2.44621100	3.32420100	0.16172100
C	-0.00235300	5.20111900	-0.03468200	0.01741000	5.17628500	-0.02027500
C	-4.15112600	-1.07458100	-1.22792700	-4.03650200	-1.16943800	1.12171600
C	-3.36642000	-1.28499700	-2.36512700	-3.11728800	-1.52117100	2.11552200
C	-3.71438100	-2.33985800	-3.20608100	-3.35083100	-2.69505700	2.82960500
C	-4.81759000	-3.16579900	-2.92815300	-4.47767700	-3.49464700	2.57729500
C	-5.60060300	-2.94528800	-1.79876400	-5.40463000	-3.12508700	1.60501200
C	-5.27397200	-1.89170900	-0.93670100	-5.19065200	-1.95416600	0.87227700
C	-5.85868900	-1.37983800	0.28525200	-5.94509600	-1.27551600	-0.16203200
C	-5.06664900	-0.27300400	0.68607100	-5.22322300	-0.10175300	-0.49601400
N	-4.03293300	-0.09408300	-0.23784900	-4.05808200	-0.04352000	0.28516800
C	-6.95724900	-1.75817200	1.06608600	-7.13647000	-1.57123500	-0.83097200
C	-7.24631800	-1.04168800	2.22396300	-7.58855900	-0.70632500	-1.82483600
C	-6.44413800	0.04593900	2.61120900	-6.85180200	0.44167100	-2.15977400
C	-5.34533400	0.44412900	1.85281100	-5.66236000	0.75884500	-1.50655400
C	5.05732500	-0.27951800	-0.69296200	5.23647700	-0.10394600	0.46217300
C	5.32365400	0.42024500	-1.87307400	5.70340800	0.78803700	1.43241600
C	6.41527100	0.01167200	-2.63631200	6.92567000	0.50636800	2.04038200
C	7.22243600	-1.06926100	-2.24074800	7.66363600	-0.64024200	1.70528600
C	6.94567900	-1.76849100	-1.06940000	7.18065300	-1.54004400	0.75756200
C	5.85454000	-1.37947500	-0.28343000	5.95820700	-1.27826400	0.13300700
C	5.28269400	-1.87336900	0.95192700	5.16760800	-2.00010700	-0.84401800
C	4.16192300	-1.05299800	1.24195700	3.99138700	-1.24138300	-1.06591700
N	4.03273800	-0.08769500	0.23843900	4.03629500	-0.08377600	-0.26943500
C	5.61913500	-2.91332600	1.82670500	5.36977000	-3.19038500	-1.54780500
C	4.84772900	-3.11726100	2.96713700	4.40847300	-3.60494000	-2.46711900
C	3.74631600	-2.28835200	3.24339200	3.25983200	-2.83034100	-2.69555100
C	3.38870500	-1.24687200	2.38991300	3.03701300	-1.63876100	-2.00749800

H	2.79093400	4.33951600	0.13728000	2.78434800	4.33983400	-0.27875100
H	4.47193500	2.52320300	0.27605900	4.49438400	2.51956300	-0.42085300
H	1.40374800	-0.47642100	0.05891000	1.43245000	-0.50372900	-0.00586800
H	-1.40428600	-0.47851100	-0.03661900	-1.45347700	-0.49232900	0.05612100
H	-4.47274000	2.51484500	-0.32497100	-4.48379500	2.57377000	0.35999800
H	-2.79405300	4.33458400	-0.20843100	-2.73740100	4.36920300	0.18032000
H	0.84651800	5.58577900	0.53644100	0.96499700	5.54852600	0.37344600
H	0.06142200	5.58049300	-1.06295700	-0.12322300	5.55803000	-1.03870500
H	-0.91665200	5.58381500	0.42621200	-0.79234700	5.54577100	0.61309400
H	-2.51720200	-0.64703400	-2.58765600	-2.25550100	-0.89852300	2.32696800
H	-3.11890100	-2.52466300	-4.09616700	-2.64690900	-2.99081000	3.60266200
H	-5.06048000	-3.98143600	-3.60329700	-4.63169100	-4.40299100	3.15282300
H	-6.45710000	-3.58111900	-1.58946900	-6.28611200	-3.73446600	1.42348500
H	-7.57446100	-2.60348600	0.77267600	-7.69772300	-2.46843300	-0.58335100
H	-8.09690100	-1.32598500	2.83700800	-8.51412700	-0.92369300	-2.35033900
H	-6.68198400	0.58775200	3.52278900	-7.21270800	1.09853000	-2.94656600
H	-4.72469100	1.27968400	2.16014800	-5.09270700	1.64054100	-1.77643700
H	4.69914400	1.25056100	-2.18673100	5.13070100	1.66578600	1.70805000
H	6.64345400	0.53989800	-3.55827600	7.30919100	1.18873200	2.79394100
H	8.06717100	-1.36198800	-2.85789900	8.61328900	-0.83136300	2.19682700
H	7.56671700	-2.60868500	-0.76942400	7.74183600	-2.43807600	0.51320700
H	6.47421500	-3.55145000	1.61858800	6.26845100	-3.77960100	-1.38554400
H	5.09836000	-3.92217200	3.65225500	4.55212500	-4.52927700	-3.01928200
H	3.15993300	-2.46019100	4.14207300	2.52805100	-3.16046600	-3.42761100
H	2.54082100	-0.60662600	2.61100200	2.15645700	-1.03778300	-2.20191400

Table S14. Optimized geometries (in Å) and energies (in hartree) of *p*-CzNF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1589.3242			Energy = -1589.101242		
C	-1.12829300	-0.01603400	0.15637700	1.13487700	0.19567600	-0.01104100
C	-2.47515900	0.00208500	0.52338800	2.45479400	0.55033000	0.04675400
C	-3.42915600	0.03302000	-0.49829100	3.43377100	-0.51380000	0.05547700
C	-3.04390100	0.04042000	-1.85448200	3.02851800	-1.87304200	0.03358700
C	-1.69956800	0.00969700	-2.20806100	1.69788100	-2.22920200	0.00137300
C	-0.72384800	-0.01224700	-1.20592400	0.69317400	-1.19148000	-0.02629400
C	0.72183600	-0.03275200	-1.20694400	-0.68969900	-1.19265900	-0.06997100
C	1.12781100	-0.05180600	0.15474700	-1.13323200	0.19423100	-0.08822500
N	-0.00001300	-0.05869200	0.96618500	0.00051600	1.00103300	-0.07724700
C	1.69656700	-0.03550100	-2.21025200	-1.69368000	-2.23089800	-0.08747700
C	3.04156200	-0.05796300	-1.85846400	-3.02466200	-1.87567100	-0.09247600
C	3.42847300	-0.05793500	-0.50270900	-3.43198500	-0.51614500	-0.09393900

C	2.47521000	-0.04712000	0.52028800	-2.45518800	0.54794800	-0.09662100
C	0.00198700	-0.03233100	2.41426000	-0.00438300	2.44647600	-0.06853200
C	5.76003800	0.86987000	-0.59488700	-5.77470000	-0.72757800	0.77093400
C	5.58970700	2.01031500	-1.38490500	-5.62746200	-1.64847500	1.81243400
C	6.71352500	2.79086100	-1.64727000	-6.76641900	-1.99727400	2.53599800
C	7.97746600	2.45266900	-1.13350300	-8.02081100	-1.43714800	2.24258400
C	8.13802800	1.32338900	-0.33609900	-8.15650500	-0.50039100	1.22023600
C	7.02512800	0.52147900	-0.05645500	-7.02933700	-0.13577600	0.47827600
C	6.83051600	-0.67950200	0.72863600	-6.80903400	0.80458000	-0.60224600
C	5.45444600	-1.01195700	0.63714200	-5.42987900	0.74374700	-0.92528600
N	4.81020400	-0.06615600	-0.16907600	-4.80026200	-0.18950200	-0.08615800
C	7.68834700	-1.49322200	1.47791900	-7.65162800	1.65508500	-1.32353500
C	7.17295100	-2.61887000	2.11391900	-7.11724000	2.42319000	-2.35608500
C	5.80960200	-2.94164300	2.00093300	-5.75345900	2.33396300	-2.68039000
C	4.93376200	-2.14841100	1.26266100	-4.89348500	1.49076500	-1.97876400
C	-5.43914800	1.01964600	0.64310100	5.40750600	0.73990700	0.95098300
C	-4.89991900	2.14738500	1.26869600	4.84357800	1.47161500	2.00079400
C	-5.76279700	2.95476000	2.00688600	5.68391500	2.30819200	2.73352100
C	-7.13125700	2.65427600	2.11973700	7.05481200	2.40509900	2.44336300
C	-7.66491000	1.53706800	1.48388300	7.61632000	1.65160700	1.41437100
C	-6.82044700	0.70942200	0.73468800	6.79386600	0.80828600	0.66210500
C	-7.03447200	-0.48821500	-0.05043800	7.04284900	-0.11820000	-0.42429500
C	-5.77515400	-0.85680000	-0.58905000	5.79732100	-0.70955300	-0.75433700
N	-4.81047600	0.06355900	-0.16309400	4.80094500	-0.18448600	0.08540000
C	-8.16000300	-1.27226900	-0.33014900	8.18851400	-0.47118700	-1.14315100
C	-8.01751800	-2.40379700	-1.12783000	8.08002600	-1.39612500	-2.17947000
C	-6.75922900	-2.76188400	-1.64206000	6.83468100	-1.95592600	-2.50966200
C	-5.62309300	-1.99939000	-1.37969400	5.67766500	-1.61853400	-1.80968500
H	-2.79432200	-0.01454100	1.55978300	2.78502800	1.58215800	0.03387000
H	-3.81291900	0.08752900	-2.61814900	3.79412100	-2.64067800	0.08621600
H	-1.41377100	0.01965000	-3.25634400	1.40345600	-3.27336700	0.01534700
H	1.40973900	-0.03186900	-3.25829900	-1.39892800	-3.27482200	-0.11103900
H	3.81002900	-0.08723200	-2.62353900	-3.79054000	-2.64362700	-0.13504900
H	2.79515100	-0.01540100	1.55604000	-2.78469600	1.57869300	-0.04261000
H	0.88108900	-0.56319300	2.78852200	-0.86098900	2.81166100	-0.64245700
H	-0.88567200	-0.54640200	2.79179100	0.90545400	2.81776300	-0.54815300
H	0.01281200	0.99199800	2.80895600	-0.06074900	2.85686100	0.94876800
H	4.61567100	2.28183500	-1.77803200	-4.65951400	-2.07061600	2.05797500
H	6.60650100	3.68140100	-2.26080000	-6.67705400	-2.71372300	3.34799000
H	8.83410500	3.08163700	-1.35849800	-8.88964500	-1.73074800	2.82474300
H	9.11414400	1.06838900	0.06850800	-9.12384700	-0.05315600	1.00686100
H	8.74483500	-1.25027500	1.55749100	-8.71125900	1.70928200	-1.08783600

H	7.82891600	-3.25712300	2.69905500	-7.76190300	3.08847000	-2.92333800
H	5.42783500	-3.83055000	2.49607500	-5.35872900	2.92675500	-3.50108000
H	3.88472800	-2.40972300	1.17069400	-3.84680800	1.40934700	-2.24952900
H	-3.84670300	2.39134900	1.17697200	3.79110800	1.38341400	2.24575100
H	-5.36661800	3.83725900	2.50216400	5.26780300	2.88929900	3.55198400
H	-7.77677800	3.30320800	2.70474600	7.68369300	3.06461300	3.03456400
H	-8.72522500	1.31139600	1.56346500	8.68122800	1.71139000	1.20534900
H	-9.13192500	-1.00186400	0.07456500	9.14925500	-0.02422600	-0.90129400
H	-8.88409100	-3.01902800	-1.35277600	8.96346300	-1.68056300	-2.74392800
H	-6.66656100	-3.65375300	-2.25599900	6.76693000	-2.66300600	-3.33188400
H	-4.65351900	-2.28595100	-1.77325900	4.71702800	-2.04031000	-2.08305200

Table S15. Optimized geometries (in Å) and energies (in hartree) of *m*-CzPF in the ground and lowest triplet excited states.

	S_0 state Energy = -1875.9218			T_1 state Energy = -1875.687982		
C	-1.27847800	3.15184900	-0.39192600	-1.25074400	3.16153300	-0.26046500
C	-2.65964900	3.30932000	-0.51256400	-2.62007800	3.32420100	-0.30280100
C	-3.49421700	2.19217200	-0.50365200	-3.47920100	2.22140700	-0.15198300
C	-2.94870600	0.90509400	-0.37470800	-2.92599300	0.89797900	0.02298800
C	-1.56488900	0.73669200	-0.25808700	-1.56963100	0.69575200	0.03789100
C	-0.72691600	1.85564000	-0.27098100	-0.67495900	1.81059100	-0.11321400
C	0.73946200	1.86329000	-0.14251900	0.71274800	1.78918500	-0.21658400
C	1.29073800	3.16503200	-0.17082500	1.30484500	3.11968200	-0.42659200
P	0.01402800	4.45829700	-0.45313400	0.04367300	4.46158900	-0.41010600
C	1.57711700	0.75160800	-0.01355900	1.58814600	0.65056500	-0.15446300
C	2.95735800	0.93513100	0.12243000	2.93991900	0.81412000	-0.32820300
C	3.50182600	2.22901900	0.10645600	3.50294400	2.11612900	-0.57785900
C	2.67112500	3.33647800	-0.06177600	2.66501300	3.24440700	-0.62325000
C	-0.13790000	5.22246900	1.25343000	0.16653500	5.04021400	1.38064700
C	3.68573900	-1.18278700	1.25660500	3.67014500	-1.47991200	-1.06060500
C	2.76164500	-1.29170100	2.29937900	2.67642200	-1.83921800	-1.97522200
C	2.87850400	-2.38237200	3.15861700	2.79367000	-3.07473300	-2.60907100
C	3.89221300	-3.34135700	2.99179900	3.87252100	-3.93493400	-2.34487300
C	4.81785900	-3.21993000	1.95960900	4.86727400	-3.56555800	-1.44337400
C	4.72341900	-2.13335600	1.08230900	4.77435600	-2.32908400	-0.79592000
C	5.50591700	-1.69781700	-0.05566100	5.61966100	-1.63784900	0.15630800
C	4.91567900	-0.49737100	-0.52660800	4.99757800	-0.39372500	0.43060000
N	3.80904700	-0.19024200	0.27549400	3.81542100	-0.29931500	-0.31528800
C	6.62771500	-2.21833300	-0.71118300	6.81600600	-1.96831700	0.80049500
C	7.13802500	-1.54796200	-1.81902800	7.36941800	-1.06726400	1.70730100

C	6.53220500	-0.36692400	-2.28090900	6.72991600	0.15254800	1.98362500
C	5.41504400	0.17297700	-1.64685200	5.53463800	0.50376200	1.35865000
C	-4.87599000	-0.43559000	0.51323500	-4.94013100	-0.46183700	-0.58157200
C	-5.33469900	0.36762600	1.56087900	-5.36928200	0.15880700	-1.75893500
C	-6.42227000	-0.09082200	2.30158000	-6.51538700	-0.34147200	-2.37474200
C	-7.03854400	-1.32071900	2.01401900	-7.20909900	-1.44243000	-1.84615400
C	-6.56861500	-2.12229600	0.97777800	-6.76022700	-2.07395200	-0.68823100
C	-5.47687400	-1.68579500	0.21819500	-5.61611700	-1.58812800	-0.04825900
C	-4.73665100	-2.25759300	-0.88735700	-4.87460400	-2.00734600	1.12409900
C	-3.71276800	-1.33414900	-1.21887800	-3.77543800	-1.12183000	1.25600600
N	-3.80398200	-0.22809000	-0.36399300	-3.82527200	-0.17670000	0.21853900
C	-4.85737300	-3.44508100	-1.61864500	-5.05623900	-3.02915300	2.06156700
C	-3.97129600	-3.69154200	-2.66319200	-4.15355400	-3.15100500	3.11493400
C	-2.97150600	-2.75847800	-2.98753200	-3.07949700	-2.25464700	3.24150600
C	-2.82889300	-1.56928000	-2.27564300	-2.87505600	-1.23016900	2.31903200
H	-3.09457400	4.29873600	-0.63046700	-3.05203300	4.31394200	-0.43172600
H	-4.56776400	2.30470600	-0.61600800	-4.55356400	2.35510300	-0.10519200
H	-1.16191300	-0.26479800	-0.14277700	-1.17698900	-0.31103300	0.13511600
H	1.17682700	-0.25741400	-0.02446500	1.18694600	-0.33743500	0.04629900
H	4.57252100	2.35620700	0.23006200	4.56560300	2.20379000	-0.77190400
H	3.10803200	4.33153000	-0.09340100	3.10523800	4.22011600	-0.81606100
H	0.73154700	5.86337100	1.43256000	1.07077900	5.64865500	1.49351500
H	-1.03116900	5.85508300	1.27959900	-0.69905200	5.67279900	1.60679200
H	-0.20296100	4.47117200	2.04533600	0.20034200	4.20788700	2.09013200
H	1.98193800	-0.55079800	2.44197500	1.84401300	-1.17862300	-2.19091400
H	2.16998200	-2.48930100	3.97551500	2.03152600	-3.37564000	-3.32261100
H	3.95429100	-4.18154100	3.67748100	3.93154200	-4.89368700	-2.85200100
H	5.60753400	-3.95675900	1.83757800	5.70840800	-4.22574900	-1.24858700
H	7.09099300	-3.13726200	-0.36134900	7.30344200	-2.91896000	0.60076200
H	8.00888400	-1.94168100	-2.33530300	8.29853800	-1.31293900	2.21355700
H	6.93914400	0.13729600	-3.15327000	7.16889300	0.83537800	2.70587600
H	4.94698700	1.07934600	-2.01642900	5.03563300	1.43767300	1.59389200
H	-4.85883100	1.31397100	1.79590800	-4.82526600	0.99360800	-2.18730200
H	-6.79770800	0.51710900	3.12033000	-6.87087800	0.12683500	-3.28841400
H	-7.88586400	-1.64872400	2.60936700	-8.09696900	-1.81050200	-2.35216200
H	-7.03949200	-3.07806900	0.76284000	-7.28789400	-2.93726600	-0.29146800
H	-5.63657000	-4.16279900	-1.37538500	-5.89462300	-3.71479500	1.97116500
H	-4.05411200	-4.61025100	-3.23681100	-4.28177500	-3.94262300	3.84755500
H	-2.29479000	-2.96442400	-3.81237100	-2.39024300	-2.35930500	4.07485000
H	-2.06093300	-0.84968600	-2.53941500	-2.04685100	-0.53888300	2.42801300

Table S16. Optimized geometries (in Å) and energies (in hartree) of *p*-CzPF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1875.9206			Energy = -1875.694241		
C	1.29106700	0.04772800	0.55287900	1.28466800	0.52899700	0.26616000
C	2.67244800	0.09873700	0.72484400	2.64227500	0.62560000	0.42814900
C	3.51796500	-0.14536600	-0.36625800	3.50886000	-0.33409300	-0.17078800
C	2.96873100	-0.47013300	-1.61673700	2.94928000	-1.41834700	-0.92268800
C	1.58914700	-0.55281300	-1.78223200	1.59685900	-1.55319300	-1.06999400
C	0.73583200	-0.28466400	-0.70488500	0.69648900	-0.58724700	-0.48118900
C	-0.73278500	-0.29474500	-0.70349200	-0.69333100	-0.57963300	-0.49856500
C	-1.29047200	0.02460600	0.55648100	-1.28750900	0.54782100	0.22672300
P	0.00024100	0.26261800	1.84736700	-0.00296100	1.67481500	0.91799800
C	-1.58438300	-0.56961400	-1.78050900	-1.58919100	-1.54214500	-1.09960900
C	-2.96468000	-0.52343600	-1.60789300	-2.94274900	-1.41056100	-0.95827900
C	-3.51637500	-0.19324500	-0.35970500	-3.50837800	-0.31999500	-0.22090700
C	-2.67191600	0.07481500	0.72661800	-2.64697600	0.65070300	0.36804800
C	-0.01276200	2.12481500	2.06516600	0.02840600	3.01933400	-0.40177700
C	-5.80892800	0.63336900	-0.96057300	-5.78310100	-1.23635100	0.28249200
C	-5.53646100	1.52808800	-1.99914100	-5.49650800	-2.55100500	0.66154800
C	-6.61358300	2.19235200	-2.58235900	-6.56609100	-3.37112800	1.01692600
C	-7.93122800	1.97919000	-2.14244400	-7.88730500	-2.89456600	1.01105500
C	-8.19462300	1.09738400	-1.09826200	-8.16328600	-1.57464800	0.66001300
C	-7.13070600	0.41719600	-0.49437500	-7.10810800	-0.73319900	0.29654900
C	-7.04173600	-0.53032200	0.59718600	-7.03177200	0.66414100	-0.08166300
C	-5.66920000	-0.85081000	0.75355100	-5.66379300	0.95361800	-0.31454300
N	-4.92513200	-0.14030800	-0.19749400	-4.90370000	-0.20669900	-0.09174800
C	-7.99008800	-1.13312500	1.43183600	-7.99077300	1.66503500	-0.26056300
C	-7.56486900	-2.04210900	2.39618800	-7.58043400	2.93044300	-0.67509900
C	-6.20191000	-2.35883900	2.52794800	-6.22405000	3.19482300	-0.92613200
C	-5.23727100	-1.77316400	1.71067200	-5.24917900	2.21302100	-0.75740500
C	5.63960700	1.03124900	0.27905700	5.59105300	-0.01174200	1.18450000
C	5.17129200	2.28703100	0.67531700	5.08840100	0.09411700	2.48448900
C	6.10982600	3.22440000	1.10191200	6.00274000	0.28498800	3.51911100
C	7.48287500	2.92590000	1.13051700	7.38354500	0.35659300	3.27198400
C	7.94432100	1.67792500	0.72198900	7.87986400	0.22512100	1.97665900
C	7.02271700	0.71798700	0.28796000	6.98310100	0.03491300	0.92162100
C	7.15032700	-0.63546400	-0.21092300	7.14931700	-0.16122700	-0.50511700
C	5.84003500	-1.09073900	-0.50567800	5.85137500	-0.31694600	-1.05306600
N	4.92629500	-0.07246700	-0.20526000	4.90255300	-0.22739400	-0.02130700
C	8.23984300	-1.48956800	-0.41772700	8.26422900	-0.19952700	-1.34700500
C	8.01245400	-2.77403800	-0.90308500	8.07423600	-0.38188000	-2.71541000

C	6.70576800	-3.21391100	-1.17592300	6.78030100	-0.51057700	-3.24625200
C	5.60383000	-2.38408200	-0.97980100	5.65245200	-0.47310300	-2.42793400
H	3.10998900	0.31055000	1.69627300	3.07981500	1.45447900	0.97785700
H	3.63295500	-0.64782400	-2.45652500	3.62108100	-2.16199700	-1.33967600
H	1.18375800	-0.80841000	-2.75758100	1.19612200	-2.40104300	-1.61809300
H	-1.17749900	-0.83093200	-2.75371700	-1.18536000	-2.36629600	-1.68067400
H	-3.62835200	-0.75766500	-2.43409000	-3.61344000	-2.11695500	-1.43725800
H	-3.10974900	0.32734800	1.68812400	-3.08670500	1.45336900	0.95350900
H	0.87024700	2.41856800	2.64208100	0.92184700	3.63645600	-0.25620200
H	-0.01788400	2.66007500	1.11160700	0.03405200	2.61014000	-1.41648000
H	-0.89878100	2.40680300	2.64315800	-0.85096700	3.66024900	-0.27397200
H	-4.52127700	1.70610400	-2.33819500	-4.47749400	-2.92039800	0.69166000
H	-6.42666600	2.89177500	-3.39275400	-6.36870500	-4.39807100	1.31165800
H	-8.74911700	2.51142700	-2.61968000	-8.69889600	-3.55883100	1.29371000
H	-9.21306500	0.94143900	-0.75200100	-9.18390700	-1.20157700	0.67684600
H	-9.04554300	-0.89691500	1.32387600	-9.04301400	1.45604500	-0.08662300
H	-8.29138600	-2.51531400	3.05057200	-8.31580300	3.71740900	-0.81554000
H	-5.89008300	-3.07787000	3.28062600	-5.92517300	4.18280200	-1.26531400
H	-4.18852900	-2.03196300	1.81235000	-4.20723300	2.42041700	-0.97415100
H	4.11386100	2.52855900	0.64679800	4.02584400	0.02004400	2.68725300
H	5.76967500	4.20755800	1.41594500	5.63572500	0.37421900	4.53777000
H	8.18865000	3.67838600	1.47051600	8.07001500	0.50636000	4.10034000
H	9.00739700	1.45181000	0.73508800	8.94985000	0.26133800	1.78965000
H	9.24994200	-1.15429900	-0.19698000	9.26501400	-0.08016000	-0.94036600
H	8.85018100	-3.44545100	-1.06852000	8.93284200	-0.41453200	-3.37991300
H	6.54741100	-4.22372400	-1.54475100	6.65124200	-0.63483300	-4.31787800
H	4.59744400	-2.73538800	-1.18216100	4.65619100	-0.55112400	-2.84894000

Table S17. Optimized geometries (in Å) and energies (in hartree) of *m*-CzOF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1569.8704			Energy = -1569.636603		
C	-3.39281700	2.42636200	0.20531400	3.41596600	2.36675300	-0.22461300
C	-3.05301700	1.05836300	0.17532000	3.03090200	0.97929300	-0.15200200
C	-1.71737100	0.65487700	0.08816800	1.71164200	0.58834900	-0.08580900
C	-0.72441500	1.63749800	0.04300600	0.69894200	1.60984300	-0.08351200
C	-1.09586500	2.99514700	0.06253300	1.12654700	3.00570300	-0.14534400
C	-2.41553600	3.41785100	0.13738400	2.42740000	3.39940800	-0.21182900
C	1.09639000	2.99510000	-0.06661600	-1.08150700	3.01574500	-0.03043700
C	0.72497500	1.63746800	-0.04580000	-0.68433800	1.62869500	0.00352500
C	1.71793100	0.65480400	-0.08989900	-1.71608300	0.63028800	0.07129100
C	3.05360200	1.05819600	-0.17731200	-3.03802100	1.05153700	0.12150800

C	3.39335800	2.42618500	-0.20866500	-3.38416100	2.42443400	0.10196800
C	2.41606000	3.41772800	-0.14178900	-2.37272600	3.43813400	0.00872800
O	0.00024800	3.82388600	-0.00245600	0.03428100	3.83783700	-0.11678700
C	6.53014200	0.33217100	2.57793200	-6.62062300	0.39386700	-2.50494700
C	7.35780200	-0.73728700	2.19467500	-7.46902300	-0.64227100	-2.07859700
C	7.07366700	-1.47813900	1.05106800	-7.16716800	-1.38109900	-0.93743100
C	5.95452200	-1.14192200	0.28045500	-6.01082600	-1.07385400	-0.21229000
C	5.13737500	-0.05213800	0.67598100	-5.17349200	-0.01484200	-0.64815600
C	5.41031700	0.68843000	1.82919700	-5.46207000	0.71932400	-1.80256000
C	4.21802700	-0.91212700	-1.21377900	-4.20975600	-0.89117400	1.21070100
C	5.36834100	-1.69015200	-0.92511300	-5.39658800	-1.63155600	0.97493700
C	5.71568600	-2.74693300	-1.77484100	-5.74878100	-2.66719800	1.84767900
C	4.92565700	-3.00856000	-2.89048100	-4.92731400	-2.94560300	2.93653800
C	3.79565800	-2.21978400	-3.16737900	-3.76134800	-2.19399600	3.16239300
C	3.42689700	-1.16247600	-2.33819000	-3.38632800	-1.15950900	2.30768800
N	4.08519800	0.08157500	-0.23697200	-4.08418800	0.09277900	0.22203900
C	-3.79911000	-2.21112400	3.17354000	3.52370700	-2.66742200	-2.76138300
C	-4.92942700	-2.99993100	2.89801200	4.71865300	-3.37073700	-2.54015800
C	-5.71834400	-2.74106900	1.78093900	5.62908000	-2.93556000	-1.57943900
C	-5.36962100	-1.68697500	0.92843500	5.33228100	-1.79380500	-0.83011500
C	-4.21905700	-0.90884900	1.21585400	4.11328500	-1.10533300	-1.05193300
C	-3.42893800	-1.15650000	2.34156500	3.20377600	-1.52788600	-2.02503000
C	-5.13603500	-0.05389600	-0.67730600	5.23603100	0.03648000	0.56455500
C	-5.95428600	-1.14196500	-0.27933400	6.04664600	-1.06818700	0.20216600
C	-7.07302800	-1.47955800	-1.04993600	7.26806200	-1.27070700	0.84951200
C	-7.35568300	-0.74171800	-2.19585800	7.66111100	-0.38169800	1.84876100
C	-6.52700300	0.32613500	-2.58140400	6.83575900	0.69367900	2.21413000
C	-5.40755000	0.68371500	-1.83274400	5.60953200	0.91306400	1.58796100
N	-4.08456900	0.08172300	0.23613000	4.06453200	0.01651200	-0.20634300
H	-4.43876700	2.70218800	0.29063000	4.45987700	2.61458200	-0.37010000
H	-1.47255200	-0.40176100	0.04940400	1.44591000	-0.45810700	0.00518300
H	-2.66979300	4.47208900	0.15713900	2.70554600	4.44584700	-0.26166300
H	1.47306600	-0.40177600	-0.04997100	-1.47388900	-0.42623500	0.06187300
H	4.43928300	2.70198000	-0.29434300	-4.42622100	2.70833700	0.19055600
H	2.67032600	4.47194400	-0.16258600	-2.63221600	4.49023300	-0.01957200
H	6.76410500	0.89341500	3.47857900	-6.86758300	0.95144500	-3.40437400
H	8.22432400	-0.98843600	2.79969400	-8.36459600	-0.87147400	-2.64909800
H	7.71029100	-2.31006300	0.76114600	-7.81880100	-2.18953600	-0.61609800
H	4.77055400	1.50971500	2.13562600	-4.80343900	1.51101900	-2.14384100
H	6.59363300	-3.35315700	-1.56706600	-6.65484600	-3.24352600	1.67918700
H	5.18460100	-3.82698400	-3.55611900	-5.18928800	-3.74833300	3.61993400
H	3.19571800	-2.43497400	-4.04750000	-3.13625900	-2.42168100	4.02164200

H	2.55791300	-0.55240000	-2.56243400	-2.48695200	-0.58062100	2.48859100
H	-3.20002100	-2.42418400	4.05475800	2.82992400	-3.01585500	-3.52130500
H	-5.18947900	-3.81622400	3.56583100	4.93591800	-4.25857100	-3.12688900
H	-6.59647900	-3.34736900	1.57417400	6.56029300	-3.47227900	-1.41905900
H	-2.55964900	-0.54642300	2.56464400	2.28249200	-0.98646700	-2.20665600
H	-7.71050600	-2.31018800	-0.75818500	7.89933200	-2.11424700	0.58336600
H	-8.22186500	-0.99397800	-2.80090100	8.60856300	-0.52867000	2.35911000
H	-6.75988900	0.88505200	-3.48377500	7.15019200	1.36442100	3.00876800
H	-4.76702900	1.50380200	-2.14081500	4.96436800	1.72902800	1.89410600

Table S18. Optimized geometries (in Å) and energies (in hartree) of *p*-CzOF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1569.8696			Energy = -1569.641188		
C	-3.40578900	-0.05082600	-0.46142500	3.41158600	-0.47850400	-0.07950700
C	-3.06171400	-0.05549800	-1.82920600	3.04581700	-1.85096100	-0.07384700
C	-1.73135300	-0.02582200	-2.23618500	1.72910300	-2.25700900	-0.05197000
C	-0.72498600	-0.01137300	-1.26390600	0.69271900	-1.25134100	-0.02384400
C	-1.09847200	-0.01943200	0.09369700	1.10392900	0.13280400	-0.03889500
C	-2.41412200	-0.02723200	0.52866400	2.39565100	0.55183100	-0.06886700
C	1.09852900	0.01975900	0.09361900	-1.10384100	0.13281900	0.03908900
C	0.72495800	0.01113000	-1.26395700	-0.69265500	-1.25134700	0.02367000
C	1.73127600	0.02516500	-2.23629400	-1.72903800	-2.25700500	0.05145400
C	3.06165800	0.05499800	-1.82939900	-3.04575000	-1.85096500	0.07337000
C	3.40582300	0.05088200	-0.46163400	-3.41154200	-0.47850500	0.07944500
C	2.41420100	0.02771900	0.52851100	-2.39559200	0.55179800	0.06907200
O	0.00005500	0.00034200	0.92259000	0.00001600	0.95994300	0.00022800
C	6.77839000	-2.70469800	-1.58328000	-6.84740600	-1.87926200	-2.46331800
C	8.01900300	-2.35547900	-1.02305900	-8.07568200	-1.27517100	-2.14903600
C	8.13195600	-1.24614500	-0.19017600	-8.15791800	-0.32198300	-1.13568000
C	6.99487400	-0.47500000	0.07737000	-7.00358400	0.01376900	-0.42332700
C	5.75435000	-0.83267400	-0.50879400	-5.77619200	-0.62302600	-0.73543000
C	5.63120800	-1.95420500	-1.33354100	-5.68176800	-1.55934400	-1.76911300
C	5.37453300	1.00722100	0.77010000	-5.34613000	0.85910400	0.93401900
C	6.75319200	0.69844200	0.89086200	-6.72879900	0.96081700	0.63945100
C	7.57410100	1.50605700	1.68638200	-7.52715000	1.84833200	1.36577100
C	7.01922200	2.60305700	2.33891700	-6.94480100	2.61294800	2.37507100
C	5.65364500	2.90292400	2.19687000	-5.57828400	2.48313700	2.67163400
C	4.81417400	2.11501400	1.41189500	-4.76208500	1.60137100	1.96487300
N	4.77284800	0.07268900	-0.08384800	-4.76591500	-0.10671000	0.09421600
C	-6.77840100	2.70444300	-1.58364900	6.84769600	-1.88010700	2.46249300
C	-8.01905600	2.35518100	-1.02354600	8.07594600	-1.27596000	2.14823500

C	-8.13202900	1.24594000	-0.19054300	8.15809300	-0.32241100	1.13521000
C	-6.99492200	0.47491500	0.07725200	7.00369200	0.01363700	0.42310900
C	-5.75434300	0.83266000	-0.50876400	5.77632200	-0.62325900	0.73515300
C	-5.63118500	1.95409200	-1.33364700	5.68197500	-1.55989400	1.76855900
C	-5.37450900	-1.00703900	0.77039600	5.34602400	0.85953800	-0.93362500
C	-6.75322600	-0.69839800	0.89092400	6.72875200	0.96110900	-0.63925800
C	-7.57415100	-1.50604800	1.68639400	7.52694800	1.84892600	-1.36537400
C	-7.01923500	-2.60291700	2.33911800	6.94438100	2.61397000	-2.37423000
C	-5.65359700	-2.90262200	2.19732700	5.57781100	2.48429400	-2.67058800
C	-4.81410200	-2.11468100	1.41240800	4.76175700	1.60221100	-1.96404700
N	-4.77279800	-0.07250300	-0.08352300	4.76595800	-0.10665100	-0.09417900
H	-3.85658100	-0.09668700	-2.56626100	3.83649900	-2.59262400	-0.12746800
H	-1.48488900	-0.02979000	-3.29395400	1.47300800	-3.31078800	-0.07447400
H	-2.66685100	-0.00224600	1.58229500	2.66070500	1.60110700	-0.03425700
H	1.48476300	0.02871200	-3.29405300	-1.47295400	-3.31079300	0.07368900
H	3.85647200	0.09591400	-2.56652600	-3.83642000	-2.59266200	0.12670700
H	2.66696800	0.00316900	1.58214400	-2.66060400	1.60109500	0.03481500
H	6.70758300	-3.58032200	-2.22286900	-6.79919500	-2.60687300	-3.26872000
H	8.89484900	-2.96067800	-1.23887400	-8.96636400	-1.54647600	-2.70841500
H	9.08972300	-0.98343500	0.25146400	-9.10487800	0.16005000	-0.90762500
H	4.67522200	-2.23745700	-1.76116100	-4.73383100	-2.01421600	-2.03334000
H	8.63246000	1.28068800	1.78870800	-8.58922300	1.93452000	1.15199800
H	7.64591400	3.23627700	2.96037900	-7.55446300	3.30770000	2.94554500
H	5.24013200	3.76872700	2.70693000	-5.14576400	3.07474100	3.47367400
H	3.76336100	2.36054100	1.30009200	-3.71346600	1.49024800	2.21643400
H	-6.70759800	3.57999200	-2.22334200	6.79957700	-2.60797800	3.26766500
H	-8.89492800	2.96027400	-1.23955200	8.96670800	-1.54752700	2.70736200
H	-9.08984100	0.98320700	0.25098700	9.10503900	0.15970300	0.90726800
H	-4.67516100	2.23734700	-1.76117800	4.73402900	-2.01476100	2.03275900
H	-8.63255500	-1.28080600	1.78854700	8.58907300	1.93500700	-1.15181800
H	-7.64594900	-3.23615700	2.96053600	7.55391800	3.30901300	-2.94448600
H	-5.24006000	-3.76831900	2.70754700	5.14514700	3.07623400	-3.47230100
H	-3.76323100	-2.36005200	1.30081600	3.71309800	1.49110600	-2.21545800

Table S19. Optimized geometries (in Å) and energies (in hartree) of *m*-CzSF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1892.8483			Energy = -1892.615952		
C	3.48260400	2.36634300	0.27115900	3.47062400	2.42096600	0.23378800
C	2.97386100	1.05377500	0.22304500	2.98738800	1.11112600	0.22147700
C	1.60105800	0.83627200	0.10989000	1.61565600	0.84433700	0.11172200
C	0.72531300	1.92888200	0.05623700	0.68571400	1.92422700	0.02628500

C	1.25453700	3.23846100	0.09462800	1.21738200	3.25534500	0.02990100
C	2.62947300	3.46144700	0.19649900	2.55826000	3.51484500	0.12286800
C	-1.25465100	3.23835300	-0.09525100	-1.32145600	3.23692400	-0.16762800
C	-0.72534000	1.92882100	-0.05656100	-0.71179000	1.88635200	-0.08891600
C	-1.60099400	0.83612500	-0.10995000	-1.59485000	0.76610600	-0.11591600
C	-2.97382100	1.05347400	-0.22315000	-2.95498200	0.96437600	-0.19924700
C	-3.48265100	2.36600300	-0.27156800	-3.53445800	2.30218000	-0.27439900
C	-2.62960900	3.46119100	-0.19717000	-2.68448900	3.42035100	-0.26718300
S	-0.00010000	4.47797200	-0.00047400	-0.08986400	4.47920400	-0.10542200
C	-6.43628200	-0.05867900	2.41901600	-6.83005700	0.25812200	1.95652600
C	-7.10273600	-1.23446400	2.03328600	-7.47316700	-0.93700300	1.60038000
C	-6.67923600	-1.95613000	0.92095700	-6.89593100	-1.80530800	0.67402000
C	-5.58276100	-1.49326100	0.18397200	-5.67714500	-1.45788200	0.08853100
C	-4.93019900	-0.29817900	0.58067500	-5.05551100	-0.23332700	0.43316200
C	-5.34254800	0.42437300	1.70352200	-5.60786400	0.62172900	1.39147600
C	-3.82846700	-1.07483200	-1.24721100	-3.67452600	-1.28934900	-1.04248200
C	-4.88109500	-1.98766000	-0.98253600	-4.79992900	-2.12810600	-0.85327800
C	-5.05537500	-3.09840800	-1.81657400	-4.89156300	-3.33492200	-1.54969000
C	-4.19291100	-3.28012400	-2.89371900	-3.86992300	-3.68643700	-2.43077000
C	-3.16273200	-2.35843500	-3.14822400	-2.77344100	-2.83341300	-2.62831700
C	-2.96656400	-1.24502400	-2.33388400	-2.66057200	-1.62382500	-1.94372400
N	-3.86523000	-0.05004600	-0.29349500	-3.83728800	-0.12522700	-0.26385500
C	3.16394700	-2.35664100	3.14975000	3.22743100	-2.24851000	3.19966500
C	4.19397900	-3.27850200	2.89525200	4.25800700	-3.17150600	2.94979400
C	5.05598300	-3.09736700	1.81764400	5.11134800	-3.00266600	1.86313000
C	4.88139300	-1.98703400	0.98311400	4.92752400	-1.90428300	1.01497100
C	3.82894500	-1.07400600	1.24783200	3.87452500	-0.98940400	1.27515400
C	2.96749400	-1.24361800	2.33495300	3.02219900	-1.14677000	2.37216800
C	4.92989000	-0.29830000	-0.58092000	4.95723700	-0.23520200	-0.56965500
C	5.58255600	-1.49324100	-0.18394800	5.61713500	-1.42398800	-0.16405900
C	6.67861700	-1.95655400	-0.92127400	6.70806800	-1.89400500	-0.90503400
C	7.10161600	-1.23545200	-2.03415600	7.11919200	-1.18646800	-2.03085400
C	6.43508300	-0.05978000	-2.42010900	6.44645100	-0.01653000	-2.42472800
C	5.34175100	0.42370400	-1.70429800	5.35952400	0.47431800	-1.70478600
N	3.86536700	-0.04966900	0.29363800	3.89964600	0.02112700	0.30934200
H	4.55239900	2.51397600	0.37740000	4.53265900	2.60599300	0.34669300
H	1.22425600	-0.18039700	0.05615100	1.27300300	-0.18409500	0.07085100
H	3.02994600	4.47010400	0.23248200	2.93759300	4.53234300	0.12780400
H	-1.22408800	-0.18049100	-0.05593400	-1.19919100	-0.23774000	-0.01051600
H	-4.55245000	2.51354900	-0.37787700	-4.59413300	2.40981100	-0.46532200
H	-3.03017600	4.46980200	-0.23340400	-3.10593600	4.41803700	-0.34921000
H	-6.77660400	0.48597900	3.29558300	-7.28305600	0.91017900	2.69782200

H	-7.95306100	-1.58365800	2.61206100	-8.42101000	-1.19545900	2.06340500
H	-7.18983200	-2.87035200	0.62950500	-7.38178900	-2.74323400	0.41944600
H	-4.82686000	1.32728500	2.01399200	-5.10116900	1.53002000	1.69626000
H	-5.85710200	-3.80722300	-1.62615300	-5.75078600	-3.98569900	-1.41229100
H	-4.31736700	-4.13929900	-3.54659700	-3.92628500	-4.62411100	-2.97585000
H	-2.50446800	-2.51331100	-3.99878400	-1.99379600	-3.11597600	-3.32980500
H	-2.17439900	-0.53339300	-2.54246700	-1.81824200	-0.96479000	-2.11631700
H	2.50604000	-2.51107700	4.00066500	2.57712200	-2.39279100	4.05834900
H	4.31868600	-4.13735700	3.54850400	4.39063500	-4.02074200	3.61418100
H	5.85757300	-3.80633800	1.62722100	5.91367000	-3.71199100	1.67648000
H	2.17544500	-0.53184400	2.54349800	2.23074600	-0.43289800	2.57506300
H	7.18930000	-2.87067000	-0.62964100	7.22400100	-2.80284000	-0.60578000
H	7.95161200	-1.58500500	-2.61319800	7.96533600	-1.54088400	-2.61278700
H	6.77502800	0.48443400	-3.29709700	6.77846800	0.51847200	-3.31052900
H	4.82599100	1.32653100	-2.01490100	4.84141100	1.37543200	-2.01571300

Table S20. Optimized geometries (in Å) and energies (in hartree) of *p*-CzSF in the ground and lowest triplet excited states.

	S_0 state			T_1 state		
	Energy = -1892.848			Energy = -1892.618943		
C	-3.50056100	0.02368100	-0.34441400	3.50418400	-0.23940000	0.27271800
C	-2.98671800	0.02666300	-1.65609400	2.96872300	-1.19668000	1.17558900
C	-1.61647800	0.00762900	-1.87772000	1.61338900	-1.34985400	1.33577100
C	-0.72623000	0.00401500	-0.79311100	0.69286700	-0.53408400	0.56938600
C	-1.25946800	0.01121900	0.51594900	1.26991500	0.43428800	-0.34741400
C	-2.63342000	0.00985500	0.75185000	2.61611200	0.59451800	-0.49742700
C	1.25948200	-0.01066700	0.51595700	-1.26985900	0.43428500	-0.34750300
C	0.72623900	-0.00506700	-0.79311000	-0.69286100	-0.53409200	0.56934800
C	1.61647700	-0.01001200	-1.87772300	-1.61341200	-1.34982500	1.33569000
C	2.98672100	-0.02874100	-1.65608200	-2.96873200	-1.19666200	1.17544700
C	3.50056200	-0.02410500	-0.34440900	-3.50415900	-0.23941400	0.27248400
C	2.63343600	-0.00898800	0.75184500	-2.61607600	0.59445100	-0.49759500
S	0.00000900	0.00101500	1.75634600	0.00002500	1.32087400	-1.22160300
C	6.06650500	-2.86544300	2.01950700	-6.08056600	3.44065500	0.29688800
C	7.43709600	-2.55557800	2.00068800	-7.44395500	3.18749900	0.07496300
C	7.90370200	-1.45394000	1.28950600	-7.90277000	1.88421300	-0.10864000
C	6.98924700	-0.65108700	0.59775000	-6.98423500	0.83149500	-0.08699500
C	5.60824500	-0.96998600	0.63964100	-5.60798700	1.10556300	0.11232900
C	5.13503400	-2.08275600	1.34020800	-5.14553000	2.40722700	0.32774900
C	5.82073100	0.87537200	-0.66957500	-5.81057500	-1.15059600	-0.08044600
C	7.12447200	0.52590600	-0.23530300	-7.11392200	-0.60763100	-0.20612700
C	8.21588700	1.30718000	-0.63234100	-8.19951200	-1.45924300	-0.42702000

C	7.99643700	2.41787100	-1.44193200	-7.97480100	-2.83097600	-0.52814400
C	6.69566200	2.75849100	-1.85053900	-6.67436900	-3.35146100	-0.42663000
C	5.59190600	1.99779900	-1.47007800	-5.57511300	-2.52243400	-0.20901700
N	4.90307000	-0.03835000	-0.13444300	-4.89297200	-0.10400100	0.11447600
C	-6.06631300	2.86690400	2.01754800	6.08060400	3.44062800	0.29710500
C	-7.43691500	2.55707600	1.99900300	7.44395400	3.18748700	0.07494700
C	-7.90358400	1.45496200	1.28860100	7.90275600	1.88421100	-0.10877900
C	-6.98918400	0.65159500	0.59737300	6.98424200	0.83148100	-0.08701900
C	-5.60816400	0.97045100	0.63899900	5.60801900	1.10554000	0.11251500
C	-5.13489700	2.08370500	1.33876300	5.14558200	2.40718900	0.32807500
C	-5.82080700	-0.87577900	-0.66897500	5.81056700	-1.15060700	-0.08043300
C	-7.12450700	-0.52595100	-0.23488100	7.11390400	-0.60764000	-0.20625300
C	-8.21598500	-1.30741600	-0.63136700	8.19945900	-1.45926400	-0.42725800
C	-7.99663800	-2.41864900	-1.44024200	7.97472000	-2.83099500	-0.52837700
C	-6.69590400	-2.75961000	-1.84869000	6.67429900	-3.35147400	-0.42672900
C	-5.59208900	-1.99873500	-1.46876600	5.57507300	-2.52243800	-0.20898400
N	-4.90305900	0.03823400	-0.13447500	4.89299700	-0.10401600	0.11468800
H	-3.67730700	0.05817200	-2.49218300	3.65517000	-1.78570600	1.77566400
H	-1.23624200	0.01146900	-2.89551900	1.22524600	-2.06609400	2.05267100
H	-3.03442900	-0.01399400	1.75968600	3.03018000	1.29327900	-1.21601600
H	1.23623100	-0.01512700	-2.89551300	-1.22531100	-2.06603700	2.05264300
H	3.67730500	-0.06133100	-2.49213700	-3.65520400	-1.78565900	1.77551900
H	3.03446800	0.01605100	1.75964600	-3.03008200	1.29321600	-1.21622200
H	5.72204100	-3.73504500	2.57257800	-5.74453800	4.46137900	0.45668700
H	8.13703900	-3.18490800	2.54284200	-8.14775200	4.01464600	0.05791600
H	8.96519600	-1.22131700	1.26697900	-8.96119000	1.68821200	-0.25842700
H	4.08011900	-2.33599600	1.35188200	-4.09874400	2.60943800	0.52483900
H	9.22110100	1.05149200	-0.30749200	-9.20384700	-1.05617600	-0.52680800
H	8.83576300	3.03102700	-1.75739500	-8.81066300	-3.50368100	-0.69731800
H	6.54315800	3.63546300	-2.47381000	-6.51685900	-4.42181300	-0.52624800
H	4.58978300	2.27437000	-1.78049400	-4.57210600	-2.93024100	-0.15458200
H	-5.72179300	3.73688400	2.56998800	5.74460200	4.46134500	0.45700800
H	-8.13681500	3.18681200	2.54074200	8.14774500	4.01463800	0.05781300
H	-8.96508800	1.22236900	1.26626100	8.96115900	1.68823700	-0.25872200
H	-4.07998000	2.33694100	1.35021500	4.09882700	2.60936400	0.52536500
H	-9.22117100	-1.05145500	-0.30664500	9.20378900	-1.05621500	-0.52716000
H	-8.83601700	-3.03195600	-1.75527100	8.81056200	-3.50370300	-0.69763700
H	-6.54347800	-3.63698700	-2.47140700	6.51677500	-4.42182500	-0.52633500
H	-4.58999700	-2.27552700	-1.77907600	4.57206500	-2.93022600	-0.15443400