Supporting Information

for

Optimizing Triazine-Based Thermally Activated Delayed Fluorescence Molecules for Enhanced Organic Light-Emitting Diode Applications

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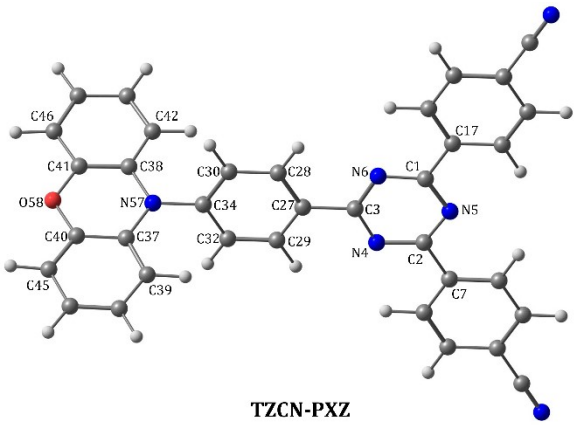

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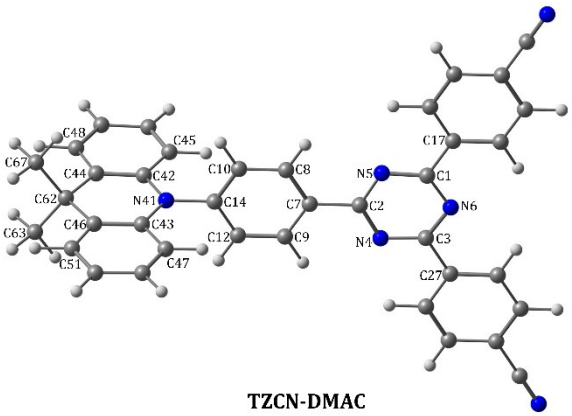

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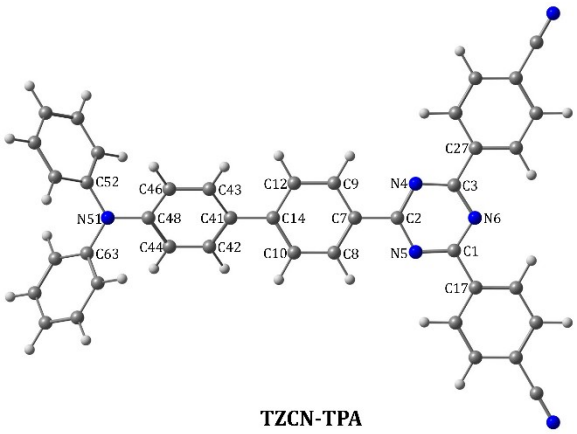

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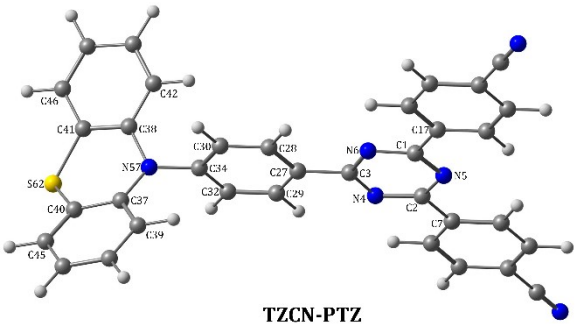

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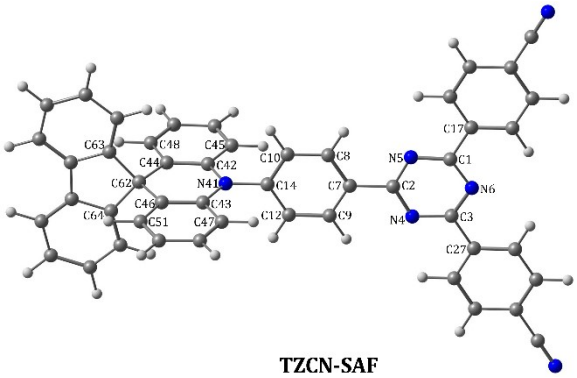

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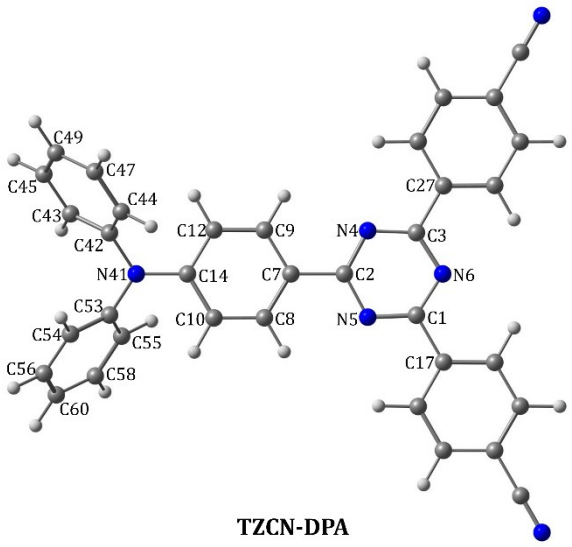

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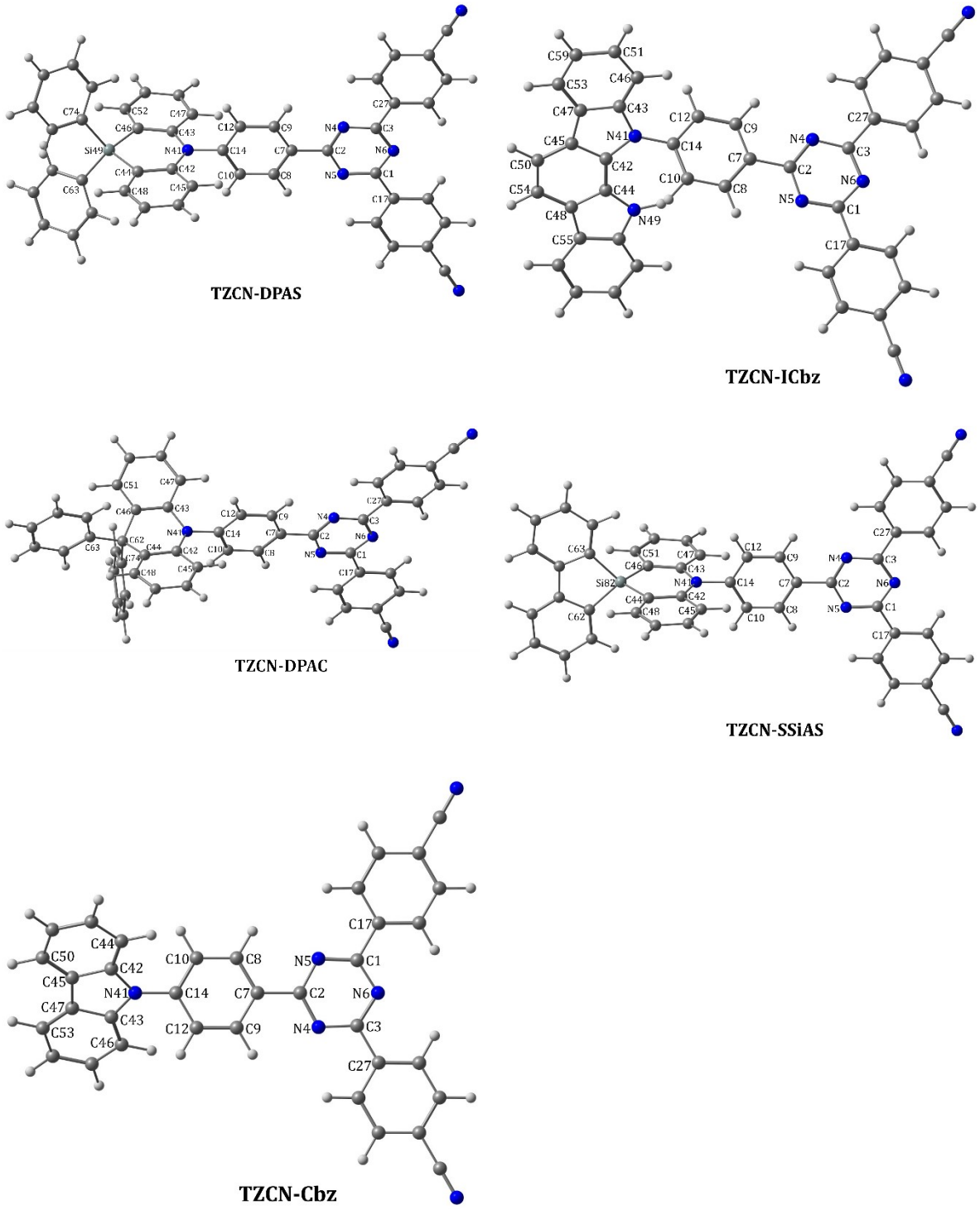


Figure S1. Atom labeling scheme used for defining bond lengths and dihedral angles.

Table S1. Calculated bond lengths and dihedral angles for the ground-state (S_0) geometries of the studied molecules in the gas phase and in toluene (PCM).

TZCN-PXZ	**Bond Length (Å)**	
Bond	**Gas Phase**	**Solvent Phase**
C41-C38	1.407	1.407
C40-C37	1.407	1.407
C41-O58	1.380	1.381
C40-O58	1.380	1.381
C38-N57	1.413	1.410
C37-N57	1.413	1.410
C41-C46	1.387	1.387
C40-C45	1.387	1.387
C38-C42	1.399	1.399
C37-C39	1.399	1.399
N57-C34	1.426	1.430
C34-C30	1.401	1.400
C34-C32	1.401	1.400
C30-C28	1.390	1.391
C32-C29	1.390	1.391
C28-C27	1.404	1.404
C29-C27	1.404	1.404
C27-C3	1.480	1.481
C3-N6	1.343	1.342
C3-N4	1.343	1.342
N6-C1	1.339	1.339
N4-C2	1.339	1.339
C1-N5	1.341	1.341
C2-N5	1.341	1.341
C1-C17	1.484	1.485
C2-C7	1.484	1.485
Dihedral Angle (°)		
C38-N57-C34-C30	72.54	80.37
C37-N57-C34-C32	72.63	80.43
C28-C27-C3-N6	-0.75	-0.43
C29-C27-C3-N4	-0.75	-0.42

TZCN-DMAC	Bond Length (Å)	
Bond	**Gas Phase**	**Solvent Phase**
C44-C42	1.410	1.410
C46-C43	1.410	1.410
C44-C62	1.533	1.533
C46-C62	1.533	1.533
C42-N41	1.409	1.408
C43-N41	1.409	1.408
C44-C48	1.401	1.401
C46-C51	1.401	1.401
C42-C45	1.409	1.409
C43-C47	1.409	1.409
C62-C67	1.553	1.553
C62-C63	1.553	1.553
N41-C14	1.433	1.434
C14-C10	1.399	1.399
C14-C12	1.399	1.399
C10-C8	1.391	1.391
C12-C9	1.391	1.391
C8-C7	1.404	1.404
C9-C7	1.404	1.404
C7-C2	1.481	1.481
C2-N5	1.342	1.342
C2-N4	1.342	1.342
N5-C1	1.339	1.339
N4-C3	1.339	1.339
C1-N6	1.341	1.341
C3-N6	1.341	1.341
C1-C17	1.484	1.485
C3-C27	1.484	1.485
Dihedral Angle (°)		
C42-N41-C14-C10	90.00	88.97
C43-N41-C14-C12	90.00	88.97
C8-C7-C2-N5	0.00	-1.20
C9-C7-C2-N4	0.00	-1.20

TZCN-TPA	Bond Length (Å)	
Bond	**Gas Phase**	**Solvent Phase**
N51-C52	1.424	1.425
N51-C63	1.424	1.425
N51-C48	1.412	1.412
C48-C46	1.406	1.406
C48-C44	1.406	1.406
C46-C43	1.388	1.389
C44-C42	1.388	1.389
C43-C41	1.406	1.407
C42-C41	1.406	1.407
C41-C14	1.478	1.478
C14-C12	1.408	1.409
C14-C10	1.408	1.409
C12-C9	1.388	1.388
C10-C8	1.388	1.388
C9-C7	1.404	1.405
C8-C7	1.404	1.405
C7-C2	1.474	1.474
C2-N4	1.345	1.345
C2-N5	1.345	1.345
N4-C3	1.338	1.337
N5-C1	1.338	1.337
C3-N6	1.342	1.341
C1-N6	1.342	1.341
C3-C27	1.485	1.486
C1-C17	1.485	1.486
Dihedral Angle (°)		
C43-C41-C14-C12	-33.35	-32.57
C42-C41-C14-C10	-33.35	-32.57
C9-C7-C2-N4	0.00	0.09
C8-C7-C2-N5	0.00	0.09

TZCN-PTZ	Bond Length (Å)	
Bond	**Gas Phase**	**Solvent Phase**
C41-C38	1.408	1.408
C40-C37	1.408	1.408
C41-S62	1.780	1.781
C40-S62	1.780	1.781
C38-N57	1.422	1.421
C37-N57	1.422	1.421
C41-C46	1.395	1.395
C40-C45	1.395	1.395
C38-C42	1.403	1.403
C37-C39	1.403	1.403
N57-C34	1.436	1.437
C34-C30	1.401	1.401
C34-C32	1.398	1.398
C30-C28	1.391	1.391
C32-C29	1.391	1.391
C28-C27	1.404	1.404
C29-C27	1.403	1.403
C27-C3	1.481	1.481
C3-N6	1.342	1.342
C3-N4	1.342	1.342
N6-C1	1.340	1.339
N4-C2	1.340	1.339
C1-N5	1.341	1.341
C2-N5	1.341	1.341
C1-C17	1.484	1.485
C2-C7	1.484	1.485
Dihedral Angle (°)		
C38-N57-C34-C30	81.90	81.82
C37-N57-C34-C32	98.07	98.16
C28-C27-C3-N6	0.00	0.00
C29-C27-C3-N4	0.00	0.00

TZCN-SAF	Bond Length (Å)	
Bond	**Gas Phase**	**Solvent Phase**
C63-C62	1.539	1.540
C64-C62	1.539	1.540
C62-C44	1.532	1.532
C62-C46	1.532	1.532
C44-C42	1.407	1.408
C46-C43	1.407	1.408
C42-N41	1.408	1.407
C43-N41	1.408	1.407
C44-C48	1.401	1.401
C46-C51	1.401	1.401
C45-C42	1.410	1.411
C47-C43	1.410	1.411
N41-C14	1.433	1.434
C14-C10	1.399	1.399
C14-C12	1.399	1.399
C10-C8	1.391	1.391
C12-C9	1.391	1.391
C8-C7	1.404	1.404
C9-C7	1.404	1.404
C7-C2	1.481	1.481
C2-N5	1.342	1.342
C2-N4	1.342	1.342
N5-C1	1.340	1.339
N4-C3	1.340	1.339
C1-N6	1.341	1.341
C3-N6	1.341	1.341
C1-C17	1.484	1.485
C3-C27	1.484	1.485
Dihedral Angle (°)		
C42-N41-C14-C10	90.02	89.11
C43-N41-C14-C12	89.99	89.07
C8-C7-C2-N5	-0.01	-0.96
C9-C7-C2-N4	0.00	-0.96

TZCN-DPA	Bond Length (Å)	
Bond	**Gas Phase**	**Solvent Phase**
C49-C47	1.396	1.396
C60-C58	1.396	1.396
C47-C44	1.393	1.394
C58-C55	1.393	1.394
C44-C42	1.402	1.402
C55-C53	1.402	1.402
C42-C43	1.402	1.402
C53-C54	1.402	1.402
C43-C45	1.393	1.394
C54-C56	1.393	1.394
C45-C49	1.396	1.396
C56-C60	1.396	1.396
C42-N41	1.428	1.429
C53-N41	1.428	1.429
N41-C14	1.404	1.402
C14-C12	1.411	1.411
C14-C10	1.411	1.411
C12-C9	1.385	1.385
C10-C8	1.385	1.385
C9-C7	1.406	1.407
C8-C7	1.406	1.407
C7-C2	1.468	1.467
C2-N4	1.347	1.347
C2-N5	1.347	1.347
N4-C3	1.336	1.336
N5-C1	1.336	1.336
C3-N6	1.342	1.342
C1-N6	1.342	1.342
C3-C27	1.486	1.487
C1-C17	1.486	1.487
Dihedral Angle (°)		
C42-N41-C14-C12	-29.57	-28.73
C53-N41-C14-C10	-29.57	-28.73
C9-C7-C2-N4	1.16	0.85
C8-C7-C2-N5	1.16	0.85

TZCN-DPAS	Bond Length (Å)	
Bond	**Gas Phase**	**Solvent Phase**
C45-C42	1.415	1.415
N41-C14	1.440	1.441
C14-C12	1.398	1.398
C14-C10	1.398	1.398
C12-C9	1.391	1.391
C10-C8	1.391	1.391
C9-C7	1.404	1.404
C8-C7	1.404	1.404
C7-C2	1.480	1.481
C2-N4	1.342	1.342
C2-N5	1.342	1.342
N4-C3	1.339	1.339
N5-C1	1.339	1.339
C3-N6	1.341	1.341
C1-N6	1.341	1.341
C3-C27	1.484	1.485
C1-C17	1.484	1.485
Dihedral Angle (°)		
C43-N41-C14-C12	89.61	89.32
C42-N41-C14-C10	89.64	89.34
C9-C7-C2-N4	-0.54	-0.90
C8-C7-C2-N5	-0.54	-0.90

TZCN-ICbz	Bond Length (Å)	
Bond	**Gas Phase**	**Solvent Phase**
C59-C51	1.404	1.405
C54-C48	1.408	1.409
C51-C46	1.393	1.393
C48-C44	1.420	1.420
C46-C43	1.396	1.397
C44-C42	1.402	1.402
C43-C47	1.416	1.417
C42-C45	1.414	1.414
C47-C53	1.400	1.400
C45-C50	1.408	1.409
C53-C59	1.391	1.391
C50-C54	1.385	1.385
C45-C47	1.447	1.447
C43-N41	1.406	1.405
C42-N41	1.406	1.405
C44-N49	1.387	1.387
C48-C55	1.448	1.448
N41-C14	1.410	1.413
C14-C12	1.404	1.403
C14-C10	1.405	1.405
C12-C9	1.389	1.389
C10-C8	1.390	1.390
C9-C7	1.404	1.404
C8-C7	1.404	1.404
C7-C2	1.477	1.478
C2-N4	1.343	1.343
C2-N5	1.343	1.343
N4-C3	1.339	1.339
N5-C1	1.339	1.339
C3-N6	1.341	1.341
C1-N6	1.341	1.341
C3-C27	1.484	1.485
C1-C17	1.484	1.485
Dihedral Angle (°)		
C43-N41-C14-C12	-55.54	-56.29
C42-N41-C14-C10	-47.89	-49.33
C9-C7-C2-N4	1.28	2.36
C8-C7-C2-N5	1.45	2.53

TZCN-DPAC	Bond Length (Å)	
Bond	**Gas Phase**	**Solvent Phase**
C46-C43	1.411	1.411
C51-C46	1.398	1.399
C43-C47	1.404	1.405
C44-C42	1.410	1.411
C48-C44	1.398	1.399
C45-C42	1.404	1.405
C62-C46	1.539	1.539
C62-C44	1.538	1.539
N41-C43	1.411	1.411
N41-C42	1.411	1.411
C62-C63	1.546	1.547
C62-C74	1.563	1.563
N41-C14	1.433	1.434
C14-C12	1.401	1.401
C14-C10	1.398	1.398
C12-C9	1.391	1.391
C10-C8	1.391	1.391
C9-C7	1.404	1.404
C8-C7	1.403	1.403
C7-C2	1.480	1.481
C2-N4	1.342	1.342
C2-N5	1.342	1.342
N4-C3	1.339	1.339
N5-C1	1.339	1.339
C3-N6	1.341	1.341
C1-N6	1.341	1.341
C3-C27	1.484	1.485
C1-C17	1.484	1.485
Dihedral Angle (°)		
C43-N41-C14-C12	82.51	82.92
C42-N41-C14-C10	95.75	96.89
C9-C7-C2-N4	-0.38	-0.04
C8-C7-C2-N5	-0.36	-0.04

TZCN-SSiAS	Bond Length (Å)	
Bond	**Gas Phase**	**Solvent Phase**
C46-C43	1.418	1.418
C51-C46	1.408	1.408
C47-C43	1.415	1.415
C44-C42	1.418	1.418
C48-C44	1.408	1.408
C45-C42	1.415	1.415
Si82-C46	1.855	1.855
Si82-C44	1.855	1.855
N41-C43	1.420	1.420
N41-C42	1.420	1.420
Si82-C63	1.885	1.885
Si82-C62	1.885	1.885
N41-C14	1.440	1.441
C14-C12	1.398	1.398
C14-C10	1.398	1.398
C12-C9	1.391	1.391
C10-C8	1.391	1.391
C9-C7	1.404	1.404
C8-C7	1.404	1.404
C7-C2	1.481	1.481
C2-N4	1.342	1.342
C2-N5	1.342	1.342
N4-C3	1.340	1.339
N5-C1	1.340	1.339
C3-N6	1.341	1.341
C1-N6	1.341	1.341
C3-C27	1.484	1.485
C1-C17	1.484	1.485
Dihedral Angle (°)		
C43-N41-C14-C12	90.00	89.65
C42-N41-C14-C10	90.01	89.66
C9-C7-C2-N4	0.00	-0.64
C8-C7-C2-N5	0.00	-0.64

TZCN-Cbz	Bond Length (Å)	
Bond	**Gas Phase**	**Solvent Phase**
C44-C42	1.397	1.397
C43-C46	1.397	1.397
C42-C45	1.416	1.417
C43-C47	1.416	1.417
C45-C50	1.399	1.399
C47-C53	1.399	1.399
C47-C45	1.448	1.448
C42-N41	1.404	1.404
C43-N41	1.404	1.404
N41-C14	1.412	1.414
C14-C10	1.403	1.403
C14-C12	1.403	1.403
C10-C8	1.388	1.389
C12-C9	1.388	1.389
C8-C7	1.404	1.404
C9-C7	1.404	1.404
C7-C2	1.476	1.477
C2-N5	1.344	1.343
C2-N4	1.344	1.343
N5-C1	1.339	1.339
N4-C3	1.339	1.339
C1-N6	1.341	1.341
C3-N6	1.341	1.341
C1-C17	1.485	1.485
C3-C27	1.485	1.485
Dihedral Angle (°)		
C42-N41-C14-C10	-49.72	-50.26
C43-N41-C14-C12	-49.72	-50.26
C8-C7-C2-N5	1.12	1.49
C9-C7-C2-N4	1.12	1.49

Table S2. Comparison of donor-acceptor dihedral angles (°) calculated at the B3LYP/6-31G(d) and B3LYP-D3(BJ)/6-31G(d) levels in toluene (PCM) for the studied molecules.

S. No.	Molecules	Bond	B3LYP	D3(BJ)
1.	TZCN-PXZ	C38-N57-C34-C30	80.38	71.52
		C37-N57-C34-C32	80.44	71.58
2.	TZCN-DMAC	C42-N41-C14-C10	88.97	88.81
		C43-N41-C14-C12	88.97	88.81
3.	TZCN-TPA	C43-C41-C14-C12	-32.58	-32.35
		C42-C41-C14-C10	-32.58	-32.35
4.	TZCN-PTZ	C38-N57-C34-C30	81.82	80.18
		C37-N57-C34-C32	98.16	99.83
5.	TZCN-SAF	C42-N41-C14-C10	89.11	83.44
		C43-N41-C14-C12	89.08	96.57
6.	TZCN-DPA	C42-N41-C14-C12	-28.74	-28.72
		C53-N41-C14-C10	-28.74	-28.72
7.	TZCN-DPAS	C43-N41-C14-C12	89.32	92.25
		C42-N41-C14-C10	89.35	88.65
8.	TZCN-ICbz	C43-N41-C14-C12	-56.30	-54.85
		C42-N41-C14-C10	-49.34	-46.55
9.	TZCN-DPAC	C43-N41-C14-C12	82.93	85.85
		C42-N41-C14-C10	96.90	87.37
10.	TZCN-SSiAS	C43-N41-C14-C12	89.66	89.62
		C42-N41-C14-C10	89.66	89.63
11.	TZCN-Cbz	C42-N41-C14-C10	-50.26	-48.49
		C43-N41-C14-C12	-50.26	-48.49

Table S3. Calculated HOMO and LUMO energies and H-L gaps (eV) of the studied molecules in their ground (S_0) state in the gas phase.

S. No.	Molecules	HOMO	LUMO	H-L Gap
1.	TZCN-PXZ	-4.90	-2.84	2.06
2.	TZCN-DMAC	-5.10	-2.83	2.26
3.	TZCN-PTZ	-5.18	-2.86	2.32
4.	TZCN-SAF	-5.16	-2.85	2.31
5.	TZCN-DPAS	-5.32	-2.84	2.48
6.	TZCN-ICbz	-5.32	-2.86	2.46
7.	TZCN-DPAC	-5.29	-2.82	2.46
8.	TZCN-SSiAS	-5.36	-2.85	2.51

Table S4. Calculated singlet-triplet energy gaps (ΔE_{ST}, eV) of the studied molecules in the gas phase and in toluene (PCM) at the M06-2X/6-31G(d) level of theory.

S. No.	Molecules	ΔE_{ST} (eV)	
		Gas Phase	Solvent Phase
1.	TZCN-PXZ	0.096	0.033
2.	TZCN-DMAC	0.005	0.005
3.	TZCN-TPA	0.545	0.493
4.	TZCN-PTZ	0.016	0.023
5.	TZCN-SAF	0.005	0.006
6.	TZCN-DPA	0.730	0.646
7.	TZCN-DPAS	0.005	0.006
8.	TZCN-ICbz	0.300	0.280
9.	TZCN-DPAC	0.009	0.008
10.	TZCN-SSiAS	0.005	0.005
11.	TZCN-Cbz	0.481	0.447

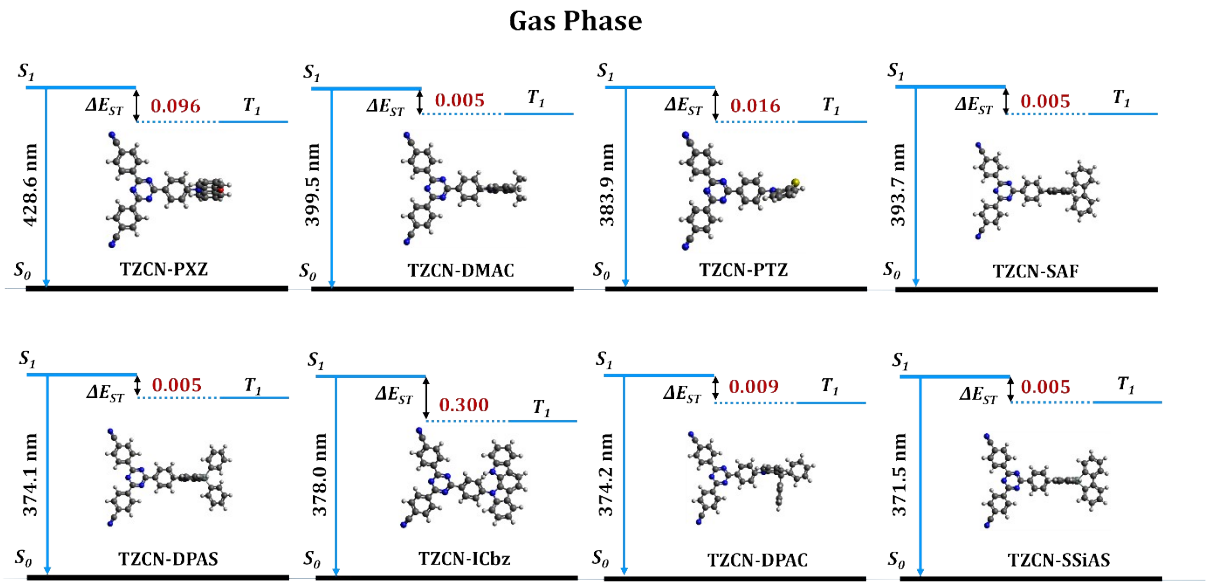
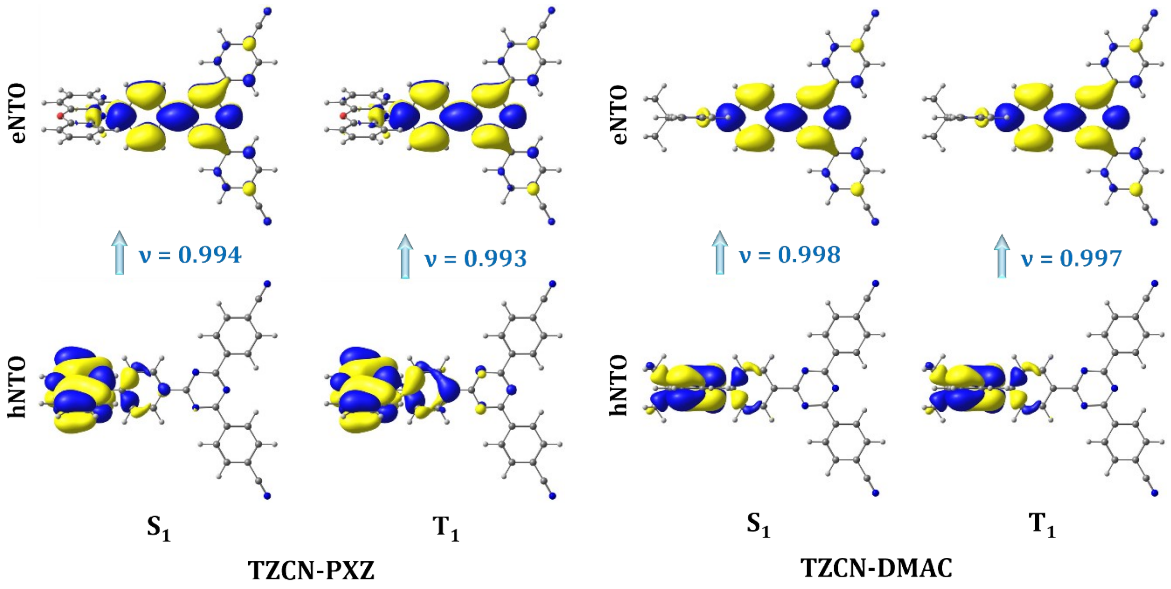
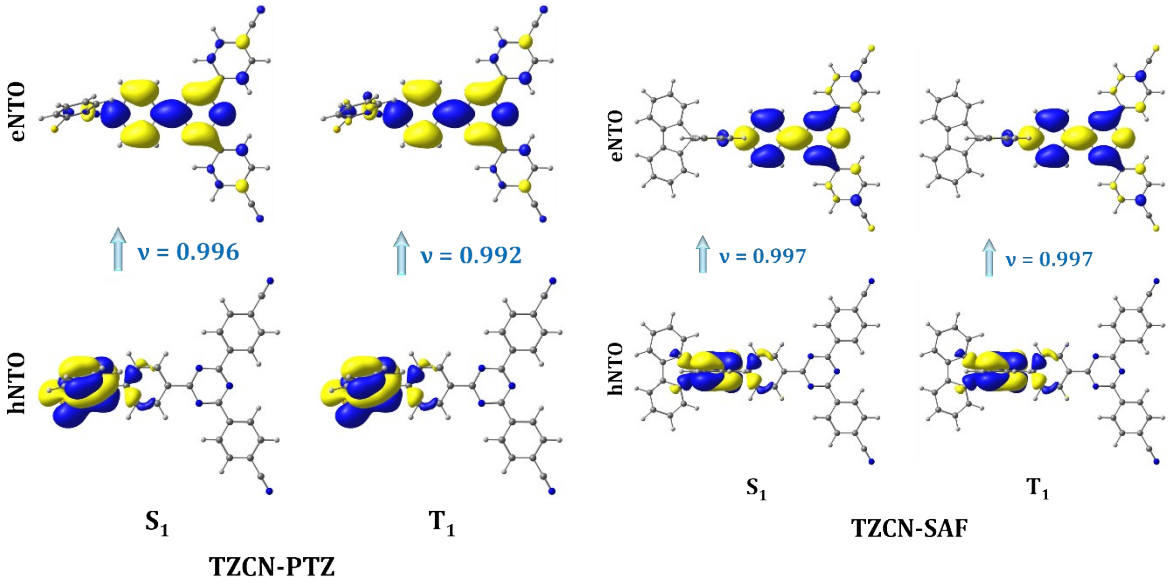
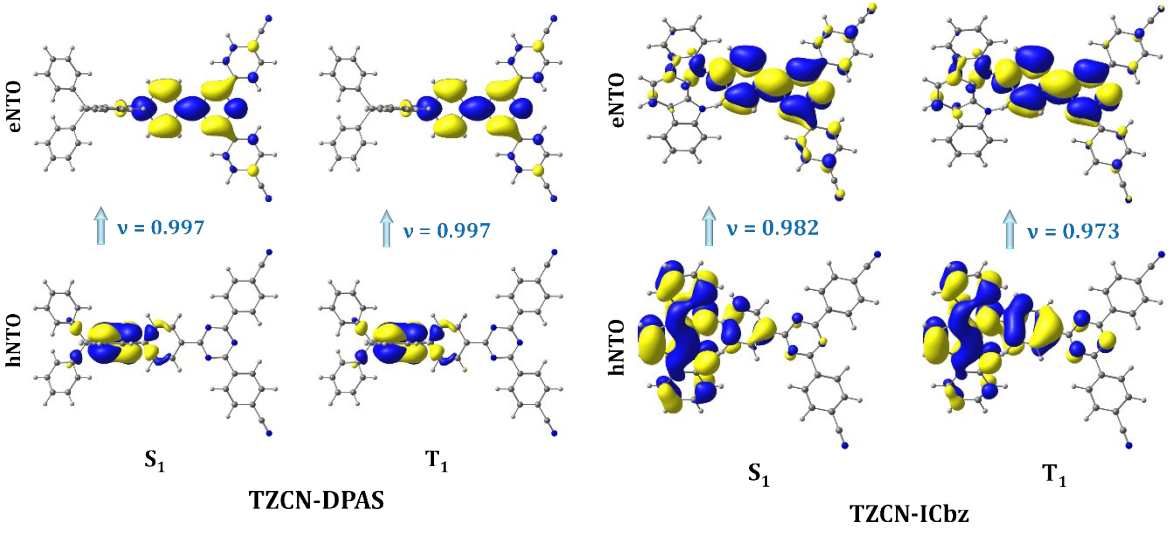


Figure S2. Calculated singlet-triplet energy gaps (ΔE_{ST}, eV) of the studied molecules in the gas phase at the M06-2X/6-31G(d) level of theory.


eNTO
ν = 0.994
ν = 0.993
hNTO
S1
T1
TZCN-PXZ
eNTO
ν = 0.998
ν = 0.997
hNTO
S1
T1
TZCN-DMAC


eNTO
ν = 0.996
ν = 0.992
hNTO
S1
T1
TZCN-PTZ
eNTO
ν = 0.997
ν = 0.997
hNTO
S1
T1
TZCN-SAF


eNTO
ν = 0.997
ν = 0.997
hNTO
S1
T1
TZCN-DPAS
eNTO
ν = 0.982
ν = 0.973
hNTO
S1
T1
TZCN-ICbz

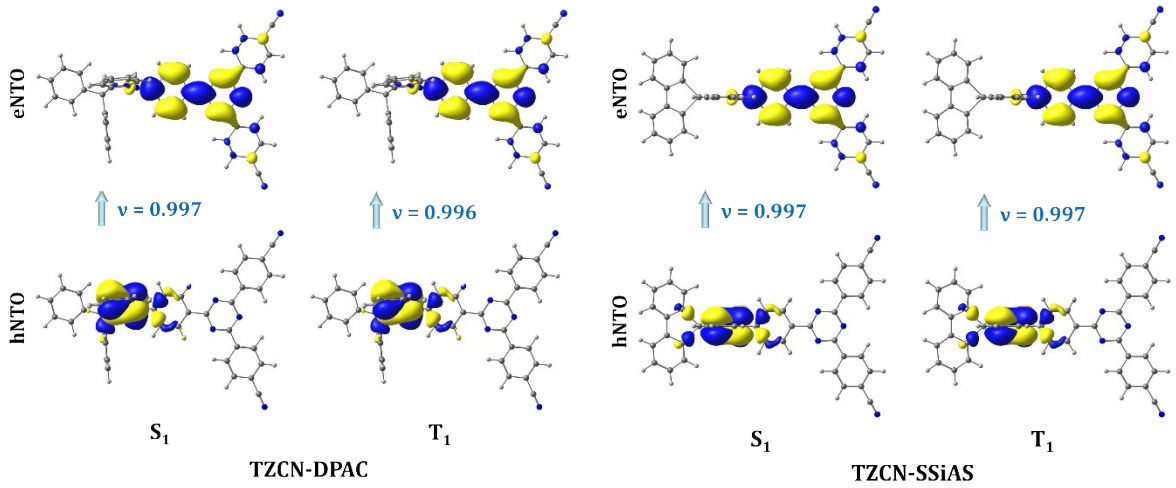


Figure S3. NTOs corresponding to the S_1 and T_1 states at their respective optimized geometries in the gas phase, calculated at the M06-2X/6-31G(d) level of theory. The hole (hNTO) and electron (eNTO) orbitals with the largest contribution (ν) are shown below and above the arrows, respectively (isosurface value = 0.02 a.u.).

Table S5. Calculated structural relaxation excited-state, RMSD, and Huang-Rhys (HR) factors of the studied molecules in the gas phase.

S. No.	Molecules	[a]Str.Relax (eV)	[b]RMSD (Å)	S Factor	Freq (cm^{-1})
1.	TZCN-PXZ	0.1023	0.0166	2.96	2434.24
2.	TZCN-DMAC	0.0001	0.0001	0	0
3.	TZCN-PTZ	0.0003	0.0002	0	0
4.	TZCN-SAF	0.0001	0.0001	0	0
5.	TZCN-DPAS	0.0003	0.2619	0	0
6.	TZCN-ICbz	0.0927	0.1010	4.12	1116.45
7.	TZCN-DPAC	0.0004	0.0022	0	0
8.	TZCN-SSiAS	0.0002	0.0001	0	0

[a]Structural relaxation energy (calculated in S_1 and T_1 optimized geometry) and [b]Root mean square deviation (RMSD) between S_1 and T_1 optimized geometry.

Table S6. Calculated spin-orbit coupling matrix elements (SOCME) between the S_1 and T_1 states at the optimized T_1 geometry using M06-2X/def2-TZVP level of theory in the gas phase.

S. No.	Molecules	ΔE_{ST} (eV)	SOCME (cm^{-1}) ($S_1 \leftarrow T_1$)	S Factor	Freq (cm^{-1})	k_{RISC} (s^{-1}) ($S_1 \leftarrow T_1$)
1.	TZCN-PXZ	0.096	0.21	2.96	2434.24	1.86×10^{4}
2.	TZCN-DMAC	0.005	0	0	0	-
3.	TZCN-PTZ	0.016	0.15	0	0	1.34×10^{6}
4.	TZCN-SAF	0.005	0	0	0	-
5.	TZCN-DPAS	0.005	0.02	0	0	2.99×10^{4}
6.	TZCN-ICbz	0.300	0.26	4.12	1116.45	3.32
7.	TZCN-DPAC	0.009	0.06	0	0	2.48×10^{5}
8.	TZCN-SSiAS	0.005	0	0	0	-

Table S7. Calculated charge transfer (CT) and local excitation (LE) contributions (%) for the S_1 and T_1 states of the studied molecules in the gas phase.

S. No.	Molecules	S_1		T_1	
		CT (%)	**LE (%)**	**CT (%)**	**LE (%)**
1.	TZCN-PXZ	93.5	6.5	89.4	10.6
2.	TZCN-DMAC	95.7	4.3	95.7	4.3
3.	TZCN-PTZ	94.9	5.1	89.2	10.8
4.	TZCN-SAF	95.7	4.3	95.6	4.4
5.	TZCN-DPAS	95.9	4.1	30.9	69.1
6.	TZCN-ICbz	88.0	12.0	76.6	23.4
7.	TZCN-DPAC	95.9	4.2	68.0	32.0
8.	TZCN-SSiAS	95.8	4.2	16.9	83.4

Table S8. Calculated charge transfer (CT) and local excitation (LE) contributions (%) for the S_1 and T_1 states of the studied molecules in toluene (PCM).

S. No.	Molecules	S_1		T_1	
		CT (%)	LE (%)	CT (%)	LE (%)
1.	TZCN-PXZ	94.9	5.1	92.7	7.3
2.	TZCN-DMAC	95.7	4.4	95.5	4.5
3.	TZCN-PTZ	94.6	5.4	15.2	84.8
4.	TZCN-SAF	95.6	4.4	95.0	5.0
5.	TZCN-DPAS	95.7	4.3	17.6	82.4
6.	TZCN-ICbz	86.7	13.3	74.6	25.4
7.	TZCN-DPAC	95.5	4.5	15.7	84.3
8.	TZCN-SSiAS	95.7	4.3	17.1	82.9

Table S9. Comparison of optical absorption energy (S_1-state) in nm using toluene solvent.

Molecules	Gaussian/ 6-31G(d)	ORCA/def2-TZVP					
	M06-2X	**M06-2X**	B3LYP	CAM-B3LYP	PBE0	WB97X	BHandHLYP
TZCN-PXZ	**414.4**	**409.6**	672.4	394.0	594.4	325.5	390.5
TZCN-DMAC	**386.4**	**384.3**	601.3	370.4	538.1	308.5	368.7
TZCN-PTZ	**369.1**	**369.9**	583.2	355.5	522.3	300.8	353.2
TZCN-SAF	**378.0**	**374.9**	578.6	362.1	520.1	302.7	359.9
TZCN-DPAS	**360.8**	**358.2**	539.8	347.4	487.0	292.6	345.5
TZCN-ICbz	**369.0**	**366.7**	554.2	356.4	500.3	311.1	356.1
TZCN-DPAC	**362.6**	**359.5**	545.9	347.9	492.2	293.2	345.6
TZCN-SSiAS	**357.7**	**355.2**	531.9	344.2	481.5	290.4	342.2

Table S10. Optimized Cartesian coordinates of S_0 geometries in toluene (PCM).

All geometries were optimized at the B3LYP/6-31G(d) level of theory in toluene.

TZCN-PXZ (S_0, Toluene)			
E = -1749.51859297 Hartree			
C	3.188899000000	1.133300000000	0.061252000000
C	3.189176000000	-1.133173000000	-0.060994000000
C	1.219488000000	-0.000176000000	0.000112000000
N	1.850239000000	-1.183677000000	-0.062506000000
N	3.903860000000	0.000151000000	0.000120000000
N	1.849950000000	1.183480000000	0.062708000000
C	3.931460000000	-2.417473000000	-0.131840000000
C	5.335289000000	-2.424977000000	-0.142197000000
C	3.235316000000	-3.635284000000	-0.189519000000
C	6.033932000000	-3.623726000000	-0.208766000000
H	5.868867000000	-1.483146000000	-0.097936000000
C	3.924608000000	-4.839406000000	-0.255973000000
H	2.151989000000	-3.624968000000	-0.181384000000
C	5.330175000000	-4.839074000000	-0.265875000000
H	7.118738000000	-3.628288000000	-0.217049000000
H	3.385450000000	-5.779733000000	-0.300327000000
C	3.930870000000	2.417787000000	0.131976000000
C	3.234430000000	3.635431000000	0.189609000000
C	5.334698000000	2.425637000000	0.142265000000
C	3.923427000000	4.839726000000	0.255962000000
H	2.151105000000	3.624849000000	0.181524000000
C	6.033048000000	3.624562000000	0.208731000000
H	5.868506000000	1.483935000000	0.098037000000
C	5.328995000000	4.839740000000	0.265802000000
H	3.384039000000	5.779923000000	0.300286000000
H	7.117853000000	3.629391000000	0.216961000000
C	-0.262175000000	-0.000351000000	0.000013000000
C	-0.973160000000	1.208310000000	0.073013000000
C	-0.972866000000	-1.209176000000	-0.073080000000
C	-2.364633000000	1.208046000000	0.076197000000
H	-0.425225000000	2.141344000000	0.133100000000
C	-2.364341000000	-1.209238000000	-0.076433000000
H	-0.424706000000	-2.142084000000	-0.133095000000
C	-3.067234000000	-0.000682000000	-0.000167000000
H	-2.916610000000	2.140757000000	0.138664000000
H	-2.916105000000	-2.142069000000	-0.138964000000
C	-5.209697000000	-0.278598000000	1.185341000000
C	-5.209754000000	0.277794000000	-1.185509000000
C	-4.578895000000	-0.546302000000	2.405547000000
C	-6.617125000000	-0.273517000000	1.155464000000
C	-6.617182000000	0.272502000000	-1.155600000000
C	-4.579023000000	0.546574000000	-2.405515000000

C	-5.327694000000	-0.813691000000	3.556467000000
H	-3.496141000000	-0.544687000000	2.456742000000
C	-7.360928000000	-0.538329000000	2.296498000000
C	-7.361050000000	0.538231000000	-2.296380000000
H	-3.496271000000	0.545106000000	-2.456752000000
C	-5.327887000000	0.814776000000	-3.556202000000
C	-6.718215000000	-0.813051000000	3.508071000000
H	-4.808985000000	-1.019385000000	4.488226000000
H	-8.443571000000	-0.522795000000	2.217602000000
C	-6.718407000000	0.813970000000	-3.507758000000
H	-8.443688000000	0.522512000000	-2.217462000000
H	-4.809230000000	1.021243000000	-4.487819000000
H	-7.306242000000	-1.019856000000	4.396886000000
H	-7.306485000000	1.021417000000	-4.396390000000
N	-4.497495000000	-0.000914000000	-0.000222000000
O	-7.324222000000	-0.001213000000	-0.000217000000
C	6.045221000000	6.080065000000	0.333995000000
N	6.626413000000	7.086460000000	0.389256000000
C	6.046700000000	-6.079220000000	-0.334172000000
N	6.628131000000	-7.085472000000	-0.389516000000

TZCN-DMAC (S_0, Toluene)

E = -1792.24608830 Hartree

C	3.620411000000	-1.134615000000	-0.016852000000
C	1.650560000000	-0.000004000000	-0.000001000000
C	3.620401000000	1.134625000000	0.016851000000
N	2.281622000000	1.185057000000	0.018467000000
N	2.281634000000	-1.185059000000	-0.018468000000
N	4.335453000000	0.000008000000	-0.000001000000
C	0.169189000000	-0.000011000000	-0.000001000000
C	-0.541878000000	-1.210115000000	-0.044306000000
C	-0.541890000000	1.210086000000	0.044303000000
C	-1.933469000000	-1.209559000000	-0.045532000000
H	0.006053000000	-2.144479000000	-0.078796000000
C	-1.933480000000	1.209518000000	0.045528000000
H	0.006033000000	2.144455000000	0.078794000000
C	-2.636111000000	-0.000024000000	-0.000002000000
H	-2.486022000000	-2.143367000000	-0.081179000000
H	-2.486042000000	2.143320000000	0.081175000000
C	4.362673000000	-2.420892000000	-0.034213000000
C	5.766501000000	-2.428838000000	-0.041362000000
C	3.666537000000	-3.640022000000	-0.042834000000
C	6.465202000000	-3.629302000000	-0.056600000000
H	6.299944000000	-1.485905000000	-0.034999000000

C	4.355871000000	-4.845881000000	-0.057832000000
H	2.583195000000	-3.629251000000	-0.037169000000
C	5.761466000000	-4.845980000000	-0.064721000000
H	7.550020000000	-3.634191000000	-0.062199000000
H	3.816734000000	-5.787252000000	-0.064080000000
C	4.362650000000	2.420909000000	0.034213000000
C	5.766478000000	2.428868000000	0.041361000000
C	3.666502000000	3.640033000000	0.042835000000
C	6.465168000000	3.629340000000	0.056600000000
H	6.299930000000	1.485941000000	0.034998000000
C	4.355825000000	4.845899000000	0.057834000000
H	2.583161000000	3.629251000000	0.037171000000
C	5.761421000000	4.846010000000	0.064723000000
H	7.549985000000	3.634238000000	0.062200000000
H	3.816679000000	5.787264000000	0.064083000000
C	6.478089000000	-6.087848000000	-0.079872000000
C	6.478031000000	6.087885000000	0.079875000000
N	7.059621000000	7.095505000000	0.092037000000
N	7.059688000000	-7.095462000000	-0.092033000000
N	-4.070572000000	-0.000030000000	-0.000002000000
C	-4.756571000000	-0.068368000000	1.228195000000
C	-4.756570000000	0.068311000000	-1.228199000000
C	-6.166749000000	-0.071698000000	1.265302000000
C	-4.029904000000	-0.132886000000	2.434277000000
C	-6.166749000000	0.071686000000	-1.265304000000
C	-4.029903000000	0.132795000000	-2.434283000000
C	-6.789364000000	-0.142573000000	2.518783000000
C	-4.681371000000	-0.202399000000	3.660281000000
H	-2.947164000000	-0.128368000000	2.410216000000
C	-6.789364000000	0.142576000000	-2.518784000000
C	-4.681371000000	0.202322000000	-3.660286000000
H	-2.947163000000	0.128242000000	-2.410224000000
C	-6.074395000000	-0.208348000000	3.712120000000
H	-7.874662000000	-0.146324000000	2.562767000000
H	-4.093005000000	-0.251436000000	4.572661000000
H	-7.874661000000	0.146371000000	-2.562766000000
C	-6.074394000000	0.208320000000	-3.712123000000
H	-4.093005000000	0.251333000000	-4.572668000000
H	-6.597775000000	-0.262329000000	4.662153000000
H	-6.597775000000	0.262314000000	-4.662155000000
C	-7.030943000000	0.000021000000	0.000003000000
C	-7.929784000000	1.264655000000	0.072127000000
H	-8.576213000000	1.339797000000	-0.808394000000

H	-8.575217000000	1.239664000000	0.956240000000
H	-7.318224000000	2.171529000000	0.123269000000
C	-7.929872000000	-1.264550000000	-0.072113000000
H	-8.576301000000	-1.339646000000	0.808410000000
H	-8.575314000000	-1.239517000000	-0.956218000000
H	-7.318375000000	-2.171466000000	-0.123260000000

TZCN-TPA (S_0, Toluene)

E = -1906.56396488 Hartree

C	-5.033196000000	1.133925000000	-0.009792000000
C	-3.060498000000	-0.000001000000	0.000005000000
C	-5.033197000000	-1.133925000000	0.009801000000
N	-3.696208000000	-1.185725000000	0.010569000000
N	-3.696208000000	1.185724000000	-0.010559000000
N	-5.750614000000	0.000000000000	0.000004000000
C	-1.585777000000	-0.000001000000	0.000005000000
C	-0.867148000000	1.207526000000	-0.008674000000
C	-0.867149000000	-1.207529000000	0.008682000000
C	0.521203000000	1.205039000000	-0.006520000000
H	-1.411299000000	2.145113000000	-0.005711000000
C	0.521202000000	-1.205043000000	0.006527000000
H	-1.411301000000	-2.145116000000	0.005720000000
C	1.251362000000	-0.000002000000	0.000003000000
H	1.051617000000	2.152129000000	0.018129000000
H	1.051616000000	-2.152133000000	-0.018123000000
C	-5.776005000000	2.421147000000	-0.020963000000
C	-7.179706000000	2.429885000000	-0.024296000000
C	-5.079829000000	3.640164000000	-0.028409000000
C	-7.878260000000	3.630606000000	-0.034782000000
H	-7.713041000000	1.486870000000	-0.018756000000
C	-5.768721000000	4.846335000000	-0.038818000000
H	-3.996462000000	3.628104000000	-0.025886000000
C	-7.174388000000	4.847191000000	-0.042052000000
H	-8.963136000000	3.635763000000	-0.037444000000
H	-5.229264000000	5.787588000000	-0.044456000000
C	-5.776007000000	-2.421147000000	0.020967000000
C	-7.179708000000	-2.429884000000	0.024296000000
C	-5.079831000000	-3.640165000000	0.028411000000
C	-7.878263000000	-3.630604000000	0.034777000000
H	-7.713042000000	-1.486869000000	0.018758000000
C	-5.768724000000	-4.846334000000	0.038816000000
H	-3.996465000000	-3.628105000000	0.025892000000

C	-7.174391000000	-4.847190000000	0.042046000000
H	-8.963138000000	-3.635761000000	0.037436000000
H	-5.229267000000	-5.787588000000	0.044452000000
C	-7.890471000000	6.089333000000	-0.052793000000
C	-7.890474000000	-6.089332000000	0.052781000000
N	-8.471493000000	-7.097396000000	0.061473000000
N	-8.471488000000	7.097397000000	-0.061489000000
C	2.729937000000	-0.000003000000	0.000002000000
C	3.463556000000	1.008302000000	-0.651927000000
C	3.463556000000	-1.008307000000	0.651931000000
C	4.852653000000	1.008492000000	-0.662813000000
H	2.938737000000	1.785608000000	-1.199929000000
C	4.852653000000	-1.008497000000	0.662816000000
H	2.938738000000	-1.785612000000	1.199935000000
C	5.575904000000	-0.000003000000	0.000000000000
H	5.386493000000	1.786402000000	-1.198309000000
H	5.386494000000	-1.786406000000	1.198312000000
N	6.988325000000	-0.000001000000	0.000001000000
C	7.709957000000	-1.228384000000	-0.037513000000
C	7.336042000000	-2.249368000000	-0.925505000000
C	8.812521000000	-1.427435000000	0.807833000000
C	8.046421000000	-3.448478000000	-0.955290000000
H	6.490661000000	-2.097174000000	-1.589204000000
C	9.528099000000	-2.622851000000	0.758544000000
H	9.103164000000	-0.642771000000	1.499241000000
C	9.147927000000	-3.641721000000	-0.118112000000
H	7.744784000000	-4.229013000000	-1.648740000000
H	10.379525000000	-2.761498000000	1.419528000000
H	9.703708000000	-4.574445000000	-0.149373000000
C	7.709952000000	1.228384000000	0.037512000000
C	7.336030000000	2.249368000000	0.925500000000
C	8.812516000000	1.427439000000	-0.807834000000
C	8.046403000000	3.448482000000	0.955283000000
H	6.490649000000	2.097172000000	1.589198000000
C	9.528088000000	2.622858000000	-0.758547000000
H	9.103163000000	0.642774000000	-1.499240000000
C	9.147909000000	3.641729000000	0.118105000000
H	7.744761000000	4.229018000000	1.648731000000
H	10.379513000000	2.761508000000	-1.419531000000
H	9.703686000000	4.574455000000	0.149365000000

TZCN-PTZ (S_0, Toluene)

E = -2072.48935009 Hartree		
C	-3.370941000000	-1.104083000000	0.000168000000
C	-3.367300000000	1.165574000000	-0.000212000000
C	-1.399598000000	0.027625000000	0.000079000000
N	-2.028299000000	1.213736000000	-0.000166000000
N	-4.083920000000	0.031802000000	-0.000054000000
N	-2.032061000000	-1.156686000000	0.000236000000
C	-4.107519000000	2.452952000000	-0.000528000000
C	-5.511356000000	2.462916000000	-0.000716000000
C	-3.409551000000	3.671070000000	-0.000646000000
C	-6.208333000000	3.664473000000	-0.001013000000
H	-6.046201000000	1.520754000000	-0.000632000000
C	-4.097184000000	4.878022000000	-0.000938000000
H	-2.326212000000	3.658837000000	-0.000502000000
C	-5.502786000000	4.880125000000	-0.001124000000
H	-7.293140000000	3.670983000000	-0.001160000000
H	-3.556672000000	5.818605000000	-0.001025000000
C	-4.115451000000	-2.389126000000	0.000386000000
C	-3.421599000000	-3.609576000000	0.000525000000
C	-5.519295000000	-2.394540000000	0.000457000000
C	-4.113148000000	-4.814260000000	0.000725000000
H	-2.338231000000	-3.600797000000	0.000472000000
C	-6.220252000000	-3.593823000000	0.000660000000
H	-6.051018000000	-1.450615000000	0.000355000000
C	-5.518757000000	-4.811796000000	0.000794000000
H	-3.575807000000	-5.756667000000	0.000829000000
H	-7.305078000000	-3.596726000000	0.000717000000
C	0.082120000000	0.025351000000	0.000082000000
C	0.790916000000	-1.186853000000	0.000294000000
C	0.795620000000	1.234040000000	-0.000132000000
C	2.182467000000	-1.189299000000	0.000293000000
H	0.241509000000	-2.120996000000	0.000462000000
C	2.187563000000	1.230941000000	-0.000133000000
H	0.250054000000	2.170391000000	-0.000299000000
C	2.889068000000	0.021237000000	0.000078000000
H	2.728746000000	-2.127766000000	0.000464000000
H	2.743858000000	2.162897000000	-0.000303000000
C	5.005577000000	-0.106890000000	1.238298000000
C	5.005594000000	-0.107663000000	-1.238048000000
C	4.360117000000	-0.618198000000	2.375303000000
C	6.360402000000	0.261211000000	1.355389000000
C	6.360429000000	0.260345000000	-1.355332000000
C	4.360146000000	-0.619634000000	-2.374759000000
C	5.042816000000	-0.757582000000	3.584474000000
H	3.315665000000	-0.899793000000	2.321246000000
C	7.047867000000	0.079535000000	2.556390000000
C	7.047921000000	0.077913000000	-2.556203000000
H	3.315681000000	-0.901155000000	-2.320562000000
C	5.042873000000	-0.759775000000	-3.583827000000

C	6.391022000000	-0.419597000000	3.681656000000
H	4.510733000000	-1.145404000000	4.448583000000
H	8.097686000000	0.354203000000	2.608804000000
C	6.391093000000	-0.421894000000	-3.681179000000
H	8.097748000000	0.352525000000	-2.608759000000
H	4.510799000000	-1.148101000000	-4.447715000000
H	6.928102000000	-0.538346000000	4.617794000000
H	6.928195000000	-0.541236000000	-4.617230000000
N	4.326230000000	0.054709000000	0.000068000000
C	-6.237521000000	-6.052532000000	0.001001000000
N	-6.820702000000	-7.059300000000	0.001168000000
C	-6.217780000000	6.123047000000	-0.001428000000
N	-6.798312000000	7.131345000000	-0.001673000000
S	7.178225000000	1.078351000000	-0.000225000000

TZCN-SAF (S_0, Toluene)

E = -2174.52771987 Hartree

C	-5.251582000000	1.134936000000	-0.003441000000
C	-3.282073000000	-0.000119000000	0.000114000000
C	-5.251875000000	-1.134667000000	0.003511000000
N	-3.912994000000	-1.185238000000	0.004558000000
N	-3.912688000000	1.185162000000	-0.004375000000
N	-5.966612000000	0.000226000000	0.000004000000
C	-1.800444000000	-0.000310000000	0.000156000000
C	-1.089352000000	1.210249000000	-0.024690000000
C	-1.089667000000	-1.211058000000	0.025024000000
C	0.302271000000	1.209577000000	-0.025723000000
H	-1.637184000000	2.145087000000	-0.044074000000
C	0.301953000000	-1.210750000000	0.026073000000
H	-1.637743000000	-2.145753000000	0.044397000000
C	1.004411000000	-0.000675000000	0.000170000000
H	0.854795000000	2.143860000000	-0.046108000000
H	0.854228000000	-2.145182000000	0.046457000000
C	-5.993720000000	2.421317000000	-0.005759000000
C	-7.397572000000	2.429346000000	-0.008232000000
C	-5.297537000000	3.640455000000	-0.004775000000
C	-8.096246000000	3.629918000000	-0.009564000000
H	-7.931049000000	1.486413000000	-0.009068000000
C	-5.986855000000	4.846411000000	-0.005982000000
H	-4.214185000000	3.629652000000	-0.002727000000
C	-7.392463000000	4.846591000000	-0.008333000000
H	-9.181071000000	3.634887000000	-0.011448000000
H	-5.447711000000	5.787795000000	-0.004976000000
C	-5.994344000000	-2.420857000000	0.005762000000
C	-7.398198000000	-2.428528000000	0.008081000000
C	-5.298472000000	-3.640173000000	0.004860000000
C	-8.097179000000	-3.628922000000	0.009339000000
H	-7.931435000000	-1.485460000000	0.008853000000

C	-5.988098000000	-4.845952000000	0.005994000000
H	-4.215117000000	-3.629647000000	0.002930000000
C	-7.393707000000	-4.845774000000	0.008188000000
H	-9.182007000000	-3.633615000000	0.011102000000
H	-5.449195000000	-5.787475000000	0.005050000000
C	-8.109043000000	6.088580000000	-0.009334000000
C	-8.110599000000	-6.087583000000	0.009112000000
N	-8.692370000000	-7.095164000000	0.009789000000
N	-8.690562000000	7.096307000000	-0.010076000000
N	2.439247000000	-0.000823000000	0.000137000000
C	3.126547000000	0.044483000000	1.227919000000
C	3.126469000000	-0.046949000000	-1.227660000000
C	4.534376000000	0.046626000000	1.267908000000
C	2.405391000000	0.087212000000	2.439964000000
C	4.534296000000	-0.049147000000	-1.267744000000
C	2.405233000000	-0.090458000000	-2.439629000000
C	5.170237000000	0.093213000000	2.515725000000
C	3.064016000000	0.133147000000	3.662098000000
H	1.322499000000	0.084192000000	2.420584000000
C	5.170072000000	-0.096637000000	-2.515569000000
C	3.063775000000	-0.137235000000	-3.661776000000
H	1.322342000000	-0.087403000000	-2.420182000000
C	4.459516000000	0.136912000000	3.709834000000
H	6.256276000000	0.094782000000	2.540216000000
H	2.480385000000	0.165681000000	4.578220000000
H	6.256110000000	-0.098239000000	-2.540132000000
C	4.459272000000	-0.141124000000	-3.709600000000
H	2.480081000000	-0.170360000000	-4.577836000000
H	4.984837000000	0.172599000000	4.659512000000
H	4.984529000000	-0.177473000000	-4.659289000000
C	5.394405000000	-0.000484000000	0.000012000000
C	6.376941000000	1.184595000000	-0.044939000000
C	6.379245000000	-1.183616000000	0.044790000000
C	6.087044000000	2.542822000000	-0.096244000000
C	7.711178000000	0.736463000000	-0.028366000000
C	6.091978000000	-2.542399000000	0.096194000000
C	7.712607000000	-0.732905000000	0.027932000000
C	7.143180000000	3.460159000000	-0.131649000000
H	5.056852000000	2.889401000000	-0.108923000000
C	8.765454000000	1.652705000000	-0.064224000000
C	7.149888000000	-3.457695000000	0.131399000000
H	5.062453000000	-2.890946000000	0.109103000000
C	8.768660000000	-1.647113000000	0.063585000000
C	8.471120000000	3.017249000000	-0.115844000000
H	6.930703000000	4.525094000000	-0.171868000000
H	9.798438000000	1.314391000000	-0.052592000000
C	8.476969000000	-3.012219000000	0.115298000000
H	6.939477000000	-4.523037000000	0.171694000000
H	9.800989000000	-1.306811000000	0.051733000000

H	9.280710000000	3.741639000000	-0.144070000000
H	9.287961000000	-3.735045000000	0.143370000000

TZCN-DPA (S_0, Toluene)

E = -1675.50739954 Hartree

C	-3.024551000000	1.129275000000	0.098178000000
C	-1.049722000000	0.000003000000	-0.000002000000
C	-3.024549000000	-1.129266000000	-0.098256000000
N	-1.689074000000	-1.182392000000	-0.100833000000
N	-1.689076000000	1.182400000000	0.100799000000
N	-3.743911000000	0.000004000000	-0.000038000000
C	0.417849000000	0.000004000000	-0.000003000000
C	1.142746000000	1.200012000000	0.120391000000
C	1.142747000000	-1.200003000000	-0.120396000000
C	2.528029000000	1.204980000000	0.123490000000
H	0.601259000000	2.133192000000	0.226976000000
C	2.528031000000	-1.204970000000	-0.123494000000
H	0.601261000000	-2.133184000000	-0.226979000000
C	3.253318000000	0.000005000000	-0.000003000000
H	3.061749000000	2.142305000000	0.232936000000
H	3.061752000000	-2.142295000000	-0.232935000000
C	-3.767866000000	2.412180000000	0.211317000000
C	-5.171470000000	2.420914000000	0.218626000000
C	-3.071822000000	3.627075000000	0.312088000000
C	-5.869929000000	3.617202000000	0.324178000000
H	-5.704790000000	1.481090000000	0.140884000000
C	-3.760326000000	4.828828000000	0.417951000000
H	-1.988464000000	3.614790000000	0.305994000000
C	-5.166033000000	4.829636000000	0.424442000000
H	-6.954847000000	3.622061000000	0.329761000000
H	-3.220592000000	5.766769000000	0.495674000000
C	-3.767863000000	-2.412175000000	-0.211358000000
C	-5.171467000000	-2.420911000000	-0.218667000000
C	-3.071816000000	-3.627072000000	-0.312093000000
C	-5.869923000000	-3.617203000000	-0.324188000000
H	-5.704788000000	-1.481086000000	-0.140951000000
C	-3.760319000000	-4.828829000000	-0.417925000000
H	-1.988458000000	-3.614785000000	-0.305999000000
C	-5.166026000000	-4.829639000000	-0.424418000000
H	-6.954842000000	-3.622064000000	-0.329773000000
H	-3.220583000000	-5.766771000000	-0.495622000000
C	-5.881699000000	6.067218000000	0.533191000000
C	-5.881690000000	-6.067224000000	-0.533135000000
N	-6.462307000000	-7.071747000000	-0.621320000000
N	-6.462318000000	7.071737000000	0.621402000000
N	4.655932000000	0.000003000000	0.000001000000
C	5.389637000000	-1.129953000000	0.476990000000
C	6.449900000000	-1.649157000000	-0.279517000000

C	5.073541000000	-1.714900000000	1.712208000000
C	7.182492000000	-2.735931000000	0.196302000000
H	6.694880000000	-1.197446000000	-1.235707000000
C	5.800418000000	-2.811927000000	2.172804000000
H	4.261309000000	-1.306431000000	2.305488000000
C	6.859572000000	-3.325662000000	1.420603000000
H	8.001786000000	-3.129030000000	-0.399435000000
H	5.545847000000	-3.256083000000	3.131257000000
H	7.428608000000	-4.175646000000	1.785981000000
C	5.389649000000	1.129955000000	-0.476982000000
C	6.449907000000	1.649153000000	0.279535000000
C	5.073574000000	1.714898000000	-1.712208000000
C	7.182514000000	2.735919000000	-0.196280000000
H	6.694873000000	1.197444000000	1.235729000000
C	5.800466000000	2.811917000000	-2.172800000000
H	4.261348000000	1.306432000000	-2.305497000000
C	6.859614000000	3.325648000000	-1.420587000000
H	8.001804000000	3.129015000000	0.399466000000
H	5.545911000000	3.256070000000	-3.131259000000
H	7.428661000000	4.175626000000	-1.785962000000

TZCN-DPAS (S_0, Toluene)

E = -2427.13040071 Hartree

C	-5.411334000000	1.135015000000	-0.009049000000
C	-3.442074000000	-0.000627000000	-0.000099000000
C	-5.412373000000	-1.134466000000	0.008956000000
N	-4.073591000000	-1.185534000000	0.009975000000
N	-4.072507000000	1.184858000000	-0.010145000000
N	-6.126846000000	0.000601000000	-0.000029000000
C	-1.960823000000	-0.001304000000	-0.000120000000
C	-1.248843000000	1.208845000000	-0.029525000000
C	-1.249950000000	-1.212113000000	0.029280000000
C	0.142703000000	1.207663000000	-0.030244000000
H	-1.796105000000	2.143949000000	-0.052562000000
C	0.141590000000	-1.212207000000	0.030040000000
H	-1.798068000000	-2.146716000000	0.052301000000
C	0.843386000000	-0.002583000000	-0.000073000000
H	0.695893000000	2.141468000000	-0.054255000000
H	0.693919000000	-2.146522000000	0.054066000000
C	-6.153050000000	2.421665000000	-0.017833000000
C	-7.556896000000	2.430194000000	-0.020906000000
C	-5.456436000000	3.640550000000	-0.022497000000
C	-8.255143000000	3.630992000000	-0.028283000000
H	-8.090696000000	1.487449000000	-0.017475000000
C	-6.145314000000	4.846738000000	-0.029771000000
H	-4.373087000000	3.629353000000	-0.020058000000
C	-7.550927000000	4.847412000000	-0.032622000000
H	-9.339967000000	3.636339000000	-0.030645000000

H	-5.605816000000	5.787916000000	-0.033147000000
C	-6.155266000000	-2.420437000000	0.017773000000
C	-7.559119000000	-2.427690000000	0.020910000000
C	-5.459760000000	-3.639955000000	0.022414000000
C	-8.258458000000	-3.627853000000	0.028328000000
H	-8.092064000000	-1.484461000000	0.017497000000
C	-6.149734000000	-4.845515000000	0.029729000000
H	-4.376401000000	-3.629739000000	0.019927000000
C	-7.555346000000	-4.844912000000	0.032645000000
H	-9.343289000000	-3.632215000000	0.030741000000
H	-5.611094000000	-5.787183000000	0.033088000000
C	-8.267087000000	6.089615000000	-0.039803000000
C	-8.272622000000	-6.086471000000	0.039869000000
N	-8.854750000000	-7.093835000000	0.045602000000
N	-8.848316000000	7.097498000000	-0.045499000000
N	2.284920000000	-0.003139000000	0.000001000000
C	2.916734000000	0.042826000000	1.271295000000
C	2.916824000000	-0.050146000000	-1.271206000000
C	4.324671000000	0.060320000000	1.442655000000
C	2.100442000000	0.072463000000	2.427805000000
C	4.324786000000	-0.066110000000	-1.442526000000
C	2.100571000000	-0.082419000000	-2.427667000000
C	4.844095000000	0.102651000000	2.751145000000
Si	5.501918000000	-0.000248000000	-0.000002000000
C	2.652799000000	0.117181000000	3.701402000000
H	1.022771000000	0.059448000000	2.337945000000
C	4.844252000000	-0.110214000000	-2.750943000000
C	2.652977000000	-0.128579000000	-3.701190000000
H	1.022884000000	-0.070474000000	-2.337819000000
C	4.037161000000	0.132821000000	3.881451000000
H	5.924872000000	0.110838000000	2.878936000000
H	1.986750000000	0.138147000000	4.560232000000
H	5.925034000000	-0.117536000000	-2.878732000000
C	4.037356000000	-0.143173000000	-3.881201000000
H	1.986955000000	-0.151630000000	-4.559987000000
H	4.471540000000	0.165688000000	4.876237000000
H	4.471776000000	-0.177295000000	-4.875926000000
C	6.600230000000	1.541641000000	-0.044793000000
C	7.814420000000	1.562967000000	-0.757956000000
C	6.191545000000	2.734752000000	0.580166000000
C	8.584702000000	2.724170000000	-0.846967000000
H	8.172626000000	0.658173000000	-1.243716000000
C	6.958794000000	3.898312000000	0.497711000000
H	5.262865000000	2.753983000000	1.145441000000
C	8.157713000000	3.895534000000	-0.218089000000
H	9.518809000000	2.713462000000	-1.403079000000
H	6.622187000000	4.805660000000	0.993072000000
H	8.757144000000	4.800000000000	-0.283349000000
C	6.607266000000	-1.537056000000	0.044707000000

C	7.822270000000	-1.552377000000	0.756631000000
C	6.203309000000	-2.732473000000	-0.578936000000
C	8.597866000000	-2.710039000000	0.845717000000
H	8.176880000000	-0.645606000000	1.241332000000
C	6.975885000000	-3.892491000000	-0.496420000000
H	5.274140000000	-2.756324000000	-1.143230000000
C	8.175520000000	-3.883775000000	0.218142000000
H	9.532483000000	-2.694708000000	1.400863000000
H	6.642859000000	-4.801717000000	-0.990757000000
H	8.779087000000	-4.785482000000	0.283453000000

TZCN-ICbz (S_0, Toluene)

E = -1959.54842648 Hartree

C	3.653705000000	1.119423000000	-0.516551000000
C	1.909306000000	-0.318698000000	-0.276492000000
C	4.019558000000	-0.989826000000	0.238138000000
N	2.718155000000	-1.297665000000	0.161621000000
N	2.335736000000	0.906494000000	-0.625869000000
N	4.536368000000	0.203916000000	-0.089534000000
C	0.463036000000	-0.606727000000	-0.379467000000
C	-0.424392000000	0.359988000000	-0.880337000000
C	-0.048705000000	-1.852917000000	0.019137000000
C	-1.784099000000	0.088650000000	-0.986924000000
H	-0.033675000000	1.317060000000	-1.206158000000
C	-1.408805000000	-2.123366000000	-0.066838000000
H	0.630013000000	-2.599357000000	0.415040000000
C	-2.290556000000	-1.154200000000	-0.570687000000
H	-2.457663000000	0.825301000000	-1.412969000000
H	-1.800136000000	-3.075937000000	0.274433000000
C	4.173201000000	2.459477000000	-0.891107000000
C	5.544956000000	2.740796000000	-0.790881000000
C	3.296957000000	3.456774000000	-1.347824000000
C	6.035737000000	3.992867000000	-1.138763000000
H	6.217981000000	1.968580000000	-0.438054000000
C	3.777713000000	4.711916000000	-1.698446000000
H	2.239061000000	3.235649000000	-1.423735000000
C	5.152392000000	4.986377000000	-1.595084000000
H	7.095964000000	4.208958000000	-1.060588000000
H	3.099498000000	5.481512000000	-2.051471000000
C	4.953561000000	-2.041029000000	0.716089000000
C	6.328238000000	-1.774889000000	0.817505000000
C	4.469626000000	-3.310634000000	1.069489000000
C	7.205696000000	-2.755250000000	1.263114000000
H	6.697963000000	-0.794127000000	0.543312000000
C	5.338716000000	-4.297765000000	1.516273000000
H	3.408168000000	-3.512045000000	0.988843000000
C	6.713818000000	-4.023938000000	1.615348000000
H	8.267847000000	-2.548537000000	1.340742000000

H	4.963390000000	-5.278476000000	1.788856000000
C	5.653804000000	6.280604000000	-1.955088000000
C	7.615304000000	-5.039466000000	2.075739000000
N	8.346723000000	-5.863570000000	2.449308000000
N	6.060614000000	7.330852000000	-2.246891000000
N	-3.672568000000	-1.434191000000	-0.671725000000
C	-4.727720000000	-0.619091000000	-0.227896000000
C	-4.226403000000	-2.516442000000	-1.376127000000
C	-4.740409000000	0.532642000000	0.573129000000
C	-5.958579000000	-1.179662000000	-0.643347000000
C	-3.586915000000	-3.563737000000	-2.044437000000
C	-5.637434000000	-2.385965000000	-1.376127000000
C	-5.985551000000	1.132634000000	0.902176000000
N	-3.722285000000	1.262365000000	1.169246000000
C	-7.188863000000	-0.579530000000	-0.306160000000
C	-4.386691000000	-4.504049000000	-2.692002000000
H	-2.505607000000	-3.645481000000	-2.068197000000
C	-6.418464000000	-3.345053000000	-2.033624000000
C	-7.201452000000	0.576651000000	0.456396000000
C	-5.679808000000	2.282388000000	1.728165000000
C	-4.267691000000	2.324696000000	1.871899000000
H	-2.738509000000	1.052197000000	1.106456000000
H	-8.119625000000	-1.029403000000	-0.639080000000
C	-5.788561000000	-4.402165000000	-2.684024000000
H	-3.912237000000	-5.329742000000	-3.214981000000
H	-7.501795000000	-3.259688000000	-2.040682000000
H	-8.142974000000	1.047565000000	0.724213000000
C	-6.460360000000	3.263627000000	2.354874000000
C	-3.628851000000	3.316838000000	2.620277000000
H	-6.383799000000	-5.152728000000	-3.196110000000
C	-5.830462000000	4.255253000000	3.101498000000
H	-7.542964000000	3.250586000000	2.259084000000
C	-4.429056000000	4.279337000000	3.231409000000
H	-2.547356000000	3.337186000000	2.722573000000
H	-6.425517000000	5.020869000000	3.591174000000
H	-3.960224000000	5.063425000000	3.819679000000

TZCN-DPAC (S_0, Toluene)

E = -2175.71101375 Hartree

C	-4.981649000000	-1.174286000000	-0.000046000000
C	-3.117980000000	0.127532000000	-0.000187000000
C	-5.179070000000	1.086620000000	-0.000094000000
N	-3.849755000000	1.253410000000	-0.000206000000
N	-3.643603000000	-1.107960000000	-0.000077000000
N	-5.792736000000	-0.105990000000	-0.000035000000
C	-1.642207000000	0.256129000000	-0.000315000000
C	-0.828469000000	-0.887767000000	0.000592000000
C	-1.039474000000	1.524665000000	-0.001382000000

C	0.558072000000	-0.766145000000	0.000513000000
H	-1.292612000000	-1.867066000000	0.001417000000
C	0.346672000000	1.645843000000	-0.001568000000
H	-1.666980000000	2.408245000000	-0.002155000000
C	1.152641000000	0.499711000000	-0.000552000000
H	1.192810000000	-1.646620000000	0.001255000000
H	0.812916000000	2.626414000000	-0.002512000000
C	-5.608702000000	-2.520571000000	-0.000039000000
C	-7.006446000000	-2.651673000000	-0.000016000000
C	-4.808211000000	-3.673921000000	-0.000088000000
C	-7.597056000000	-3.908941000000	-0.000051000000
H	-7.620753000000	-1.759259000000	0.000024000000
C	-5.389047000000	-4.935690000000	-0.000121000000
H	-3.729990000000	-3.567984000000	-0.000111000000
C	-6.789200000000	-5.059137000000	-0.000107000000
H	-8.677280000000	-4.009145000000	-0.000040000000
H	-4.769450000000	-5.826199000000	-0.000163000000
C	-6.030487000000	2.303549000000	0.000016000000
C	-7.429710000000	2.189361000000	-0.000066000000
C	-5.443068000000	3.578654000000	0.000229000000
C	-8.230262000000	3.324571000000	0.000056000000
H	-7.879002000000	1.203508000000	-0.000226000000
C	-6.234721000000	4.720019000000	0.000359000000
H	-4.362872000000	3.662197000000	0.000307000000
C	-7.635012000000	4.597885000000	0.000273000000
H	-9.311438000000	3.234963000000	-0.000011000000
H	-5.779803000000	5.704888000000	0.000534000000
C	-7.393886000000	-6.359235000000	-0.000158000000
C	-8.456621000000	5.773026000000	0.000412000000
N	-9.123340000000	6.726537000000	0.000525000000
N	-7.884602000000	-7.414177000000	-0.000203000000
N	2.584095000000	0.596386000000	-0.000832000000
C	3.270482000000	0.789451000000	-1.218568000000
C	3.270899000000	0.795247000000	1.215737000000
C	4.674685000000	0.649680000000	-1.243892000000
C	2.582020000000	1.128926000000	-2.395948000000
C	4.675162000000	0.655909000000	1.241105000000
C	2.582879000000	1.139884000000	2.391872000000
C	5.348594000000	0.910453000000	-2.442109000000
C	3.277419000000	1.358175000000	-3.579995000000
H	1.502834000000	1.223510000000	-2.383087000000
C	5.349543000000	0.922729000000	2.437733000000
C	3.278755000000	1.374999000000	3.574488000000
H	1.503643000000	1.233861000000	2.379153000000
C	4.668241000000	1.265053000000	-3.607113000000
H	6.428304000000	0.809654000000	-2.467179000000
H	2.724905000000	1.622250000000	-4.477770000000
H	6.429312000000	0.822531000000	2.462739000000
C	4.669629000000	1.282665000000	3.601353000000

H	2.726557000000	1.643022000000	4.471286000000
H	5.219500000000	1.450017000000	-4.524388000000
H	5.221266000000	1.472268000000	4.517453000000
C	5.384511000000	0.085922000000	-0.000136000000
C	6.877022000000	0.493192000000	-0.001726000000
C	7.922917000000	-0.435467000000	-0.001334000000
C	7.208724000000	1.860233000000	-0.004235000000
C	9.258439000000	-0.015605000000	-0.003247000000
H	7.704269000000	-1.497166000000	0.000464000000
C	8.535931000000	2.281143000000	-0.006109000000
H	6.413045000000	2.599728000000	-0.004700000000
C	9.571619000000	1.341335000000	-0.005602000000
H	10.050869000000	-0.759586000000	-0.002879000000
H	8.762616000000	3.344203000000	-0.007985000000
H	10.608322000000	1.667228000000	-0.007057000000
C	5.225343000000	-1.469832000000	0.004213000000
C	5.179926000000	-2.190252000000	1.207446000000
C	5.171861000000	-2.196717000000	-1.194746000000
C	5.082839000000	-3.583212000000	1.213128000000
H	5.216454000000	-1.662246000000	2.153965000000
C	5.074689000000	-3.589739000000	-1.192180000000
H	5.202128000000	-1.673934000000	-2.144369000000
C	5.027326000000	-4.291882000000	0.012539000000
H	5.046946000000	-4.112144000000	2.162187000000
H	5.032372000000	-4.123795000000	-2.138101000000
H	4.947318000000	-5.375722000000	0.015754000000

TZCN-SSiAS (S_0, Toluene)

E = -2425.93724088 Hartree

C	-5.500199000000	1.135514000000	-0.001679000000
C	-3.531163000000	-0.000375000000	-0.000034000000
C	-5.501431000000	-1.134125000000	0.001510000000
N	-4.162576000000	-1.185275000000	0.002285000000
N	-4.161290000000	1.185209000000	-0.002391000000
N	-6.215695000000	0.001083000000	-0.000079000000
C	-2.049741000000	-0.001173000000	-0.000034000000
C	-1.337753000000	1.209166000000	-0.016115000000
C	-1.339043000000	-1.212277000000	0.016053000000
C	0.053820000000	1.207935000000	-0.016718000000
H	-1.884961000000	2.144491000000	-0.028552000000
C	0.052527000000	-1.212534000000	0.016676000000
H	-1.887248000000	-2.147019000000	0.028485000000
C	0.754140000000	-0.002666000000	-0.000019000000
H	0.606962000000	2.141981000000	-0.029737000000
H	0.604670000000	-2.147173000000	0.029705000000
C	-6.241830000000	2.422185000000	-0.002167000000
C	-7.645682000000	2.430746000000	-0.002670000000
C	-5.545187000000	3.641063000000	-0.001583000000

C	-8.343901000000	3.631582000000	-0.002500000000
H	-8.179512000000	1.488013000000	-0.003134000000
C	-6.234047000000	4.847282000000	-0.001361000000
H	-4.461836000000	3.629866000000	-0.001091000000
C	-7.639658000000	4.847989000000	-0.001777000000
H	-9.428725000000	3.636962000000	-0.002846000000
H	-5.694544000000	5.788461000000	-0.000765000000
C	-6.244462000000	-2.419989000000	0.002085000000
C	-7.648323000000	-2.427030000000	0.002566000000
C	-5.549138000000	-3.639619000000	0.001606000000
C	-8.347843000000	-3.627110000000	0.002468000000
H	-8.181136000000	-1.483721000000	0.002951000000
C	-6.239304000000	-4.845090000000	0.001459000000
H	-4.465777000000	-3.629591000000	0.001135000000
C	-7.644915000000	-4.844278000000	0.001847000000
H	-9.432674000000	-3.631319000000	0.002792000000
H	-5.700823000000	-5.786853000000	0.000944000000
C	-8.355787000000	6.090240000000	-0.001359000000
C	-8.362372000000	-6.085761000000	0.001506000000
N	-8.944615000000	-7.093069000000	0.001181000000
N	-8.936959000000	7.098165000000	-0.000972000000
N	2.196012000000	-0.003329000000	0.000002000000
C	2.827971000000	0.021369000000	1.271395000000
C	2.828008000000	-0.028793000000	-1.271360000000
C	4.236123000000	0.027302000000	1.443029000000
C	2.013641000000	0.040886000000	2.429604000000
C	4.236169000000	-0.033380000000	-1.442967000000
C	2.013721000000	-0.050481000000	-2.429562000000
C	4.760523000000	0.053287000000	2.750238000000
C	2.569338000000	0.066408000000	3.702062000000
H	0.935739000000	0.036043000000	2.341439000000
C	4.760620000000	-0.060667000000	-2.750129000000
C	2.569469000000	-0.077069000000	-3.701976000000
H	0.935813000000	-0.046618000000	-2.341426000000
C	3.954621000000	0.073285000000	3.880687000000
H	5.841805000000	0.057536000000	2.872898000000
H	1.905128000000	0.080828000000	4.562436000000
H	5.841907000000	-0.064039000000	-2.872763000000
C	3.954761000000	-0.082942000000	-3.880566000000
H	1.905291000000	-0.093216000000	-4.562344000000
H	4.389562000000	0.093268000000	4.875523000000
H	4.389740000000	-0.103840000000	-4.875365000000
C	6.722140000000	1.345794000000	-0.030362000000
C	6.726750000000	-1.343275000000	0.030319000000
C	6.610831000000	2.737427000000	-0.063193000000
C	8.008333000000	0.748494000000	-0.017719000000
C	6.620200000000	-2.735284000000	0.063174000000
C	8.010890000000	-0.741572000000	0.017642000000
C	7.755260000000	3.541391000000	-0.083641000000

H	5.628906000000	3.206143000000	-0.073273000000
C	9.150601000000	1.557056000000	-0.038877000000
C	7.767374000000	-3.535322000000	0.083624000000
H	5.639885000000	-3.207358000000	0.073280000000
C	9.155923000000	-1.546222000000	0.038795000000
C	9.019521000000	2.947261000000	-0.071550000000
H	7.662612000000	4.623961000000	-0.109095000000
H	10.143530000000	1.115473000000	-0.030741000000
C	9.029593000000	-2.936866000000	0.071498000000
H	7.678432000000	-4.618202000000	0.109102000000
H	10.147343000000	-1.101253000000	0.030633000000
H	9.910789000000	3.569380000000	-0.087848000000
H	9.922984000000	-3.555933000000	0.087796000000
Si	5.402534000000	-0.001024000000	0.000008000000

TZCN-Cbz (S_0, Toluene)

E = -1674.32812742 Hartree

C	3.085422000000	-1.129027000000	0.111867000000
C	1.114606000000	0.000001000000	0.000004000000
C	3.085422000000	1.129026000000	-0.111872000000
N	1.747385000000	1.179988000000	-0.115959000000
N	1.747384000000	-1.179988000000	0.115961000000
N	3.801417000000	0.000000000000	-0.000003000000
C	-0.362731000000	0.000001000000	0.000002000000
C	-1.078236000000	-1.199482000000	0.149520000000
C	-1.078235000000	1.199484000000	-0.149517000000
C	-2.467456000000	-1.201517000000	0.157281000000
H	-0.532580000000	-2.127229000000	0.276590000000
C	-2.467456000000	1.201519000000	-0.157280000000
H	-0.532579000000	2.127230000000	-0.276587000000
C	-3.175826000000	0.000001000000	0.000000000000
H	-3.011122000000	-2.128606000000	0.304710000000
H	-3.011121000000	2.128608000000	-0.304711000000
C	3.827769000000	-2.409562000000	0.238737000000
C	5.231562000000	-2.417842000000	0.244779000000
C	3.131300000000	-3.623110000000	0.353418000000
C	5.929770000000	-3.612922000000	0.362898000000
H	5.765453000000	-1.479335000000	0.156060000000
C	3.819977000000	-4.823527000000	0.471996000000
H	2.047963000000	-3.611985000000	0.347968000000
C	5.225599000000	-4.823975000000	0.477260000000
H	7.014637000000	-3.617912000000	0.367478000000
H	3.280347000000	-5.760495000000	0.560560000000
C	3.827769000000	2.409561000000	-0.238739000000
C	5.231562000000	2.417841000000	-0.244785000000
C	3.131301000000	3.623110000000	-0.353415000000
C	5.929771000000	3.612921000000	-0.362902000000
H	5.765454000000	1.479333000000	-0.156070000000

C	3.819978000000	4.823527000000	-0.471991000000
H	2.047964000000	3.611986000000	-0.347962000000
C	5.225600000000	4.823974000000	-0.477259000000
H	7.014638000000	3.617910000000	-0.367485000000
H	3.280348000000	5.760495000000	-0.560551000000
C	5.941403000000	-6.060356000000	0.599125000000
C	5.941405000000	6.060355000000	-0.599123000000
N	6.522157000000	7.063701000000	-0.697914000000
N	6.522155000000	-7.063701000000	0.697918000000
N	-4.589871000000	0.000001000000	-0.000001000000
C	-5.412300000000	-0.834890000000	-0.773193000000
C	-5.412301000000	0.834891000000	0.773191000000
C	-5.062014000000	-1.796079000000	-1.725851000000
C	-6.768107000000	-0.530242000000	-0.493313000000
C	-5.062016000000	1.796080000000	1.725850000000
C	-6.768107000000	0.530242000000	0.493312000000
C	-6.093412000000	-2.470565000000	-2.377312000000
H	-4.024925000000	-2.009354000000	-1.960967000000
C	-7.785392000000	-1.222412000000	-1.160795000000
C	-6.093414000000	2.470565000000	2.377312000000
H	-4.024926000000	2.009356000000	1.960966000000
C	-7.785393000000	1.222411000000	1.160794000000
C	-7.442511000000	-2.194030000000	-2.097015000000
H	-5.844343000000	-3.223610000000	-3.119851000000
H	-8.828615000000	-0.999004000000	-0.953674000000
C	-7.442512000000	2.194029000000	2.097015000000
H	-5.844345000000	3.223609000000	3.119851000000
H	-8.828616000000	0.999002000000	0.953673000000
H	-8.222399000000	-2.739348000000	-2.620615000000
H	-8.222401000000	2.739345000000	2.620615000000

Table S11. Optimized Cartesian coordinates of T_1 geometries in toluene (PCM).

All geometries were optimized at the B3LYP/6-31G(d) level of theory in toluene.

TZCN-PXZ (T_1, Toluene) *E* = -1749.50792221 Hartree		
C	-3.202154000000	1.159157000000	-0.005862000000
C	-3.191519000000	-1.132643000000	0.003725000000
C	-1.229107000000	0.005222000000	-0.001116000000
N	-1.825476000000	-1.204853000000	0.004703000000
N	-3.897650000000	-0.017374000000	-0.001110000000
N	-1.820701000000	1.182405000000	-0.006681000000
C	-3.933161000000	-2.418096000000	0.008598000000
C	-5.339720000000	-2.439624000000	0.008676000000
C	-3.238666000000	-3.640914000000	0.013091000000
C	-6.034052000000	-3.640266000000	0.013090000000
H	-5.873464000000	-1.496459000000	0.005169000000
C	-3.923102000000	-4.849476000000	0.017509000000
H	-2.155526000000	-3.622640000000	0.012904000000
C	-5.329237000000	-4.860554000000	0.017540000000
H	-7.119429000000	-3.647346000000	0.013092000000
H	-3.379585000000	-5.789196000000	0.020907000000
C	-3.921330000000	2.400959000000	-0.009825000000
C	-3.237173000000	3.651975000000	-0.014177000000
C	-5.346774000000	2.436910000000	-0.009202000000
C	-3.923998000000	4.847051000000	-0.017498000000
H	-2.153557000000	3.648699000000	-0.014619000000
C	-6.035906000000	3.630112000000	-0.012538000000
H	-5.888116000000	1.498022000000	-0.005873000000
C	-5.342337000000	4.868994000000	-0.016728000000
H	-3.380676000000	5.787670000000	-0.020685000000
H	-7.122069000000	3.631189000000	-0.011863000000
C	0.272129000000	0.004523000000	-0.001068000000
C	0.983855000000	1.211502000000	-0.014126000000
C	0.979973000000	-1.204337000000	0.012219000000
C	2.376573000000	1.218463000000	-0.014201000000
H	0.427537000000	2.141145000000	-0.024201000000
C	2.374563000000	-1.214217000000	0.012980000000
H	0.421846000000	-2.132580000000	0.022065000000
C	3.057360000000	0.000295000000	-0.000413000000
H	2.928204000000	2.153822000000	-0.024528000000
H	2.923927000000	-2.151004000000	0.023589000000

C	5.206024000000	-0.018425000000	-1.200797000000
C	5.205238000000	0.019099000000	1.201305000000
C	4.557395000000	-0.035623000000	-2.452777000000
C	6.624214000000	-0.018403000000	-1.175999000000
C	6.623444000000	0.018850000000	1.177441000000
C	4.555783000000	0.038251000000	2.452831000000
C	5.307712000000	-0.051666000000	-3.614332000000
H	3.476397000000	-0.035291000000	-2.491455000000
C	7.375528000000	-0.035471000000	-2.349502000000
C	7.373987000000	0.036917000000	2.351421000000
H	3.474761000000	0.039209000000	2.490788000000
C	5.305339000000	0.055777000000	3.614854000000
C	6.716090000000	-0.051842000000	-3.568643000000
H	4.800450000000	-0.064072000000	-4.572484000000
H	8.456994000000	-0.034657000000	-2.276441000000
C	6.713746000000	0.055141000000	3.570100000000
H	8.455501000000	0.035937000000	2.279078000000
H	4.797451000000	0.070542000000	4.572642000000
H	7.288390000000	-0.064634000000	-4.489418000000
H	7.285438000000	0.069298000000	4.491233000000
N	4.513183000000	-0.000547000000	0.000040000000
O	7.306332000000	-0.000479000000	0.000954000000
C	-6.048095000000	6.099928000000	-0.019877000000
N	-6.627431000000	7.115826000000	-0.022443000000
C	-6.037448000000	-6.103950000000	0.021974000000
N	-6.611379000000	-7.117678000000	0.025551000000

TZCN-DMAC (T_1, Toluene)

E = -1792.23812067 Hartree

C	3.627497000000	-1.144556000000	-0.010691000000
C	1.657681000000	0.000001000000	-0.000001000000
C	3.627501000000	1.144565000000	0.010690000000
N	2.245325000000	1.193366000000	0.012507000000
N	2.245327000000	-1.193374000000	-0.012509000000
N	4.320412000000	-0.000005000000	0.000000000000
C	0.152329000000	0.000001000000	-0.000001000000
C	-0.556316000000	-1.206789000000	-0.031240000000
C	-0.556318000000	1.206790000000	0.031239000000
C	-1.950647000000	-1.215275000000	-0.031955000000
H	0.001458000000	-2.135174000000	-0.054896000000
C	-1.950647000000	1.215275000000	0.031954000000
H	0.001456000000	2.135176000000	0.054895000000

C	-2.632000000000	-0.000001000000	0.000000000000
H	-2.501305000000	-2.150906000000	-0.056699000000
H	-2.501306000000	2.150905000000	0.056698000000
C	4.360052000000	-2.403966000000	-0.020548000000
C	5.776168000000	-2.433650000000	-0.021074000000
C	3.670936000000	-3.641220000000	-0.029441000000
C	6.467660000000	-3.630115000000	-0.029942000000
H	6.314817000000	-1.493136000000	-0.014253000000
C	4.356826000000	-4.843191000000	-0.038232000000
H	2.587625000000	-3.630488000000	-0.028776000000
C	5.768321000000	-4.860368000000	-0.038631000000
H	7.553430000000	-3.634057000000	-0.030158000000
H	3.812996000000	-5.783170000000	-0.044770000000
C	4.360047000000	2.403961000000	0.020547000000
C	5.776170000000	2.433651000000	0.021074000000
C	3.670934000000	3.641224000000	0.029441000000
C	6.467660000000	3.630113000000	0.029943000000
H	6.314822000000	1.493138000000	0.014252000000
C	4.356825000000	4.843191000000	0.038232000000
H	2.587622000000	3.630496000000	0.028775000000
C	5.768324000000	4.860372000000	0.038632000000
H	7.553430000000	3.634053000000	0.030159000000
H	3.812994000000	5.783170000000	0.044770000000
C	6.475061000000	-6.097464000000	-0.047329000000
C	6.475062000000	6.097464000000	0.047331000000
N	7.051916000000	7.112160000000	0.054388000000
N	7.051914000000	-7.112159000000	-0.054387000000
N	-4.091579000000	-0.000001000000	0.000000000000
C	-4.759260000000	-0.042211000000	1.219134000000
C	-4.759261000000	0.042210000000	-1.219134000000
C	-6.180228000000	-0.045690000000	1.259989000000
C	-4.005264000000	-0.080621000000	2.420984000000
C	-6.180228000000	0.045690000000	-1.259988000000
C	-4.005265000000	0.080620000000	-2.420984000000
C	-6.788991000000	-0.090018000000	2.515081000000
C	-4.646585000000	-0.122330000000	3.642367000000
H	-2.925673000000	-0.076743000000	2.376987000000
C	-6.788991000000	0.090018000000	-2.515080000000
C	-4.646586000000	0.122329000000	-3.642367000000
H	-2.925674000000	0.076741000000	-2.376987000000
C	-6.047334000000	-0.127671000000	3.694627000000
H	-7.871230000000	-0.094692000000	2.580590000000
H	-4.061992000000	-0.151119000000	4.555205000000

H	-7.871231000000	0.094692000000	-2.580589000000
C	-6.047335000000	0.127671000000	-3.694626000000
H	-4.061993000000	0.151119000000	-4.555205000000
H	-6.558681000000	-0.161007000000	4.650787000000
H	-6.558683000000	0.161007000000	-4.650787000000
C	-7.033069000000	0.000000000000	0.000000000000
C	-7.932762000000	1.270848000000	0.047406000000
H	-8.576671000000	1.319477000000	-0.834634000000
H	-8.576575000000	1.253371000000	0.930823000000
H	-7.325396000000	2.180175000000	0.081450000000
C	-7.932765000000	-1.270845000000	-0.047405000000
H	-8.576674000000	-1.319472000000	0.834636000000
H	-8.576579000000	-1.253367000000	-0.930821000000
H	-7.325401000000	-2.180173000000	-0.081449000000

TZCN-TPA (T_1, Toluene)

E = -1906.55795580 Hartree

C	-1.135710000000	0.076568000000	-5.018367000000
C	0.000000000000	0.000000000000	-3.039579000000
C	1.135710000000	-0.076568000000	-5.018367000000
N	1.194644000000	-0.078822000000	-3.693219000000
N	-1.194644000000	0.078822000000	-3.693219000000
N	0.000000000000	0.000000000000	-5.753579000000
C	0.000000000000	0.000000000000	-1.594492000000
C	-1.214670000000	0.058654000000	-0.852422000000
C	1.214670000000	-0.058654000000	-0.852422000000
C	-1.211359000000	0.064969000000	0.522831000000
H	-2.151359000000	0.092063000000	-1.396487000000
C	1.211359000000	-0.064969000000	0.522831000000
H	2.151359000000	-0.092063000000	-1.396487000000
C	0.000000000000	0.000000000000	1.278570000000
H	-2.167167000000	0.084549000000	1.036373000000
H	2.167167000000	-0.084549000000	1.036373000000
C	-2.419808000000	0.165965000000	-5.762378000000
C	-2.427914000000	0.171875000000	-7.167271000000
C	-3.642251000000	0.246796000000	-5.074051000000
C	-3.623494000000	0.255384000000	-7.870285000000
H	-1.483595000000	0.110630000000	-7.694629000000
C	-4.842549000000	0.330512000000	-5.765450000000
H	-3.631429000000	0.242856000000	-3.990457000000
C	-4.841718000000	0.335190000000	-7.173420000000
H	-3.623743000000	0.259491000000	-8.955603000000

H	-5.783730000000	0.392550000000	-5.228632000000
C	2.419808000000	-0.165965000000	-5.762378000000
C	2.427914000000	-0.171875000000	-7.167271000000
C	3.642251000000	-0.246796000000	-5.074051000000
C	3.623494000000	-0.255384000000	-7.870285000000
H	1.483595000000	-0.110630000000	-7.694629000000
C	4.842549000000	-0.330512000000	-5.765450000000
H	3.631429000000	-0.242856000000	-3.990457000000
C	4.841718000000	-0.335190000000	-7.173420000000
H	3.623743000000	-0.259491000000	-8.955603000000
H	5.783730000000	-0.392550000000	-5.228632000000
C	-6.077553000000	0.420954000000	-7.891911000000
C	6.077553000000	-0.420954000000	-7.891911000000
N	7.083388000000	-0.490735000000	-8.474426000000
N	-7.083388000000	0.490735000000	-8.474426000000
C	0.000000000000	0.000000000000	2.723583000000
C	-1.157268000000	0.363928000000	3.484229000000
C	1.157268000000	-0.363928000000	3.484229000000
C	-1.163163000000	0.360579000000	4.859575000000
H	-2.051037000000	0.698122000000	2.971334000000
C	1.163163000000	-0.360579000000	4.859575000000
H	2.051037000000	-0.698122000000	2.971334000000
C	0.000000000000	0.000000000000	5.588313000000
H	-2.051079000000	0.677991000000	5.395807000000
H	2.051079000000	-0.677991000000	5.395807000000
N	0.000000000000	0.000000000000	6.988255000000
C	1.169827000000	0.370530000000	7.705890000000
C	1.937485000000	1.468665000000	7.279873000000
C	1.559935000000	-0.358807000000	8.842656000000
C	3.083723000000	1.824986000000	7.984427000000
H	1.619631000000	2.043098000000	6.416371000000
C	2.706749000000	0.010054000000	9.538840000000
H	0.974300000000	-1.215171000000	9.159419000000
C	3.473346000000	1.099943000000	9.114173000000
H	3.667025000000	2.680081000000	7.656515000000
H	3.009464000000	-0.562848000000	10.410172000000
H	4.367536000000	1.382791000000	9.661144000000
C	-1.169827000000	-0.370530000000	7.705890000000
C	-1.937485000000	-1.468665000000	7.279873000000
C	-1.559935000000	0.358807000000	8.842656000000
C	-3.083723000000	-1.824986000000	7.984427000000
H	-1.619631000000	-2.043098000000	6.416371000000
C	-2.706749000000	-0.010054000000	9.538840000000

H	-0.974300000000	1.215171000000	9.159419000000
C	-3.473346000000	-1.099943000000	9.114173000000
H	-3.667025000000	-2.680081000000	7.656515000000
H	-3.009464000000	0.562848000000	10.410172000000
H	-4.367536000000	-1.382791000000	9.661144000000

TZCN-PTZ (T_1, Toluene)

E = -2072.47534849 Hartree

C	-3.375604000000	-1.158790000000	-0.000010000000
C	-3.364500000000	1.132797000000	-0.000003000000
C	-1.401959000000	-0.005312000000	-0.000048000000
N	-1.998497000000	1.204739000000	-0.000025000000
N	-4.070938000000	0.017596000000	0.000000000000
N	-1.994095000000	-1.182513000000	-0.000034000000
C	-4.105887000000	2.418354000000	0.000006000000
C	-5.512469000000	2.440293000000	0.000023000000
C	-3.411124000000	3.641073000000	-0.000001000000
C	-6.206507000000	3.641095000000	0.000032000000
H	-6.046454000000	1.497254000000	0.000028000000
C	-4.095266000000	4.849792000000	0.000008000000
H	-2.327986000000	3.622482000000	-0.000014000000
C	-5.501422000000	4.861269000000	0.000025000000
H	-7.291889000000	3.648421000000	0.000045000000
H	-3.551495000000	5.789377000000	0.000002000000
C	-4.095088000000	-2.400522000000	-0.000009000000
C	-3.411067000000	-3.651627000000	-0.000022000000
C	-5.520536000000	-2.436369000000	0.000004000000
C	-4.098004000000	-4.846648000000	-0.000021000000
H	-2.327449000000	-3.648362000000	-0.000031000000
C	-6.209804000000	-3.629478000000	0.000005000000
H	-6.061764000000	-1.497405000000	0.000013000000
C	-5.516364000000	-4.868502000000	-0.000008000000
H	-3.554747000000	-5.787316000000	-0.000030000000
H	-7.295972000000	-3.630429000000	0.000015000000
C	0.098974000000	-0.004659000000	-0.000033000000
C	0.811293000000	-1.211517000000	-0.000047000000
C	0.807737000000	1.203865000000	-0.000009000000
C	2.204214000000	-1.217661000000	-0.000036000000
H	0.255240000000	-2.141444000000	-0.000066000000
C	2.202536000000	1.212617000000	0.000003000000
H	0.250129000000	2.132547000000	0.000000000000
C	2.886788000000	-0.000791000000	-0.000008000000

H	2.755677000000	-2.153284000000	-0.000047000000
H	2.751969000000	2.149522000000	0.000022000000
C	4.990662000000	-0.001230000000	1.236864000000
C	4.990669000000	-0.001194000000	-1.236849000000
C	4.227319000000	-0.003554000000	2.429875000000
C	6.407379000000	0.000031000000	1.362625000000
C	6.407385000000	0.000069000000	-1.362606000000
C	4.227327000000	-0.003486000000	-2.429860000000
C	4.843247000000	-0.004460000000	3.665832000000
H	3.148833000000	-0.005200000000	2.369757000000
C	7.016530000000	-0.000648000000	2.629955000000
C	7.016539000000	-0.000577000000	-2.629934000000
H	3.148841000000	-0.005133000000	-2.369742000000
C	4.843258000000	-0.004361000000	-3.665816000000
C	6.245435000000	-0.002851000000	3.776351000000
H	4.229333000000	-0.006755000000	4.559932000000
H	8.100282000000	0.000306000000	2.694325000000
C	6.245446000000	-0.002751000000	-3.776332000000
H	8.100291000000	0.000376000000	-2.694301000000
H	4.229345000000	-0.006632000000	-4.559917000000
H	6.720348000000	-0.003658000000	4.751093000000
H	6.720361000000	-0.003533000000	-4.751072000000
N	4.347567000000	-0.000121000000	0.000005000000
C	-6.222237000000	-6.099333000000	-0.000006000000
N	-6.801721000000	-7.115176000000	-0.000005000000
C	-6.209326000000	6.104813000000	0.000035000000
N	-6.783076000000	7.118670000000	0.000043000000
S	7.491187000000	0.003000000000	0.000012000000

TZCN-SAF (T_1, Toluene)

E = -2174.51862716 Hartree

C	-5.249869000000	-1.132460000000	-0.000035000000
C	-3.287029000000	0.004863000000	0.000137000000
C	-5.260045000000	1.159140000000	0.000061000000
N	-3.878523000000	1.182218000000	0.000180000000
N	-3.883805000000	-1.204880000000	0.000008000000
N	-5.955803000000	-0.016974000000	-0.000036000000
C	-1.785857000000	0.003804000000	0.000136000000
C	-1.077567000000	-1.204660000000	-0.000127000000
C	-1.073501000000	1.210301000000	0.000401000000
C	0.317178000000	-1.214376000000	-0.000143000000
H	-1.635179000000	-2.133329000000	-0.000299000000

C	0.319342000000	1.216873000000	0.000385000000
H	-1.629205000000	2.140418000000	0.000596000000
C	1.000603000000	-0.000624000000	0.000106000000
H	0.866366000000	-2.151291000000	-0.000354000000
H	0.870956000000	2.152265000000	0.000587000000
C	-5.991684000000	-2.417697000000	-0.000022000000
C	-7.398282000000	-2.439151000000	-0.000230000000
C	-5.297316000000	-3.640649000000	0.000199000000
C	-8.092711000000	-3.639717000000	-0.000211000000
H	-7.931972000000	-1.495948000000	-0.000415000000
C	-5.981867000000	-4.849133000000	0.000227000000
H	-4.214174000000	-3.622436000000	0.000340000000
C	-7.388024000000	-4.860130000000	0.000026000000
H	-9.178094000000	-3.646681000000	-0.000371000000
H	-5.438409000000	-5.788899000000	0.000400000000
C	-5.978887000000	2.401213000000	-0.000001000000
C	-7.404320000000	2.437833000000	-0.000048000000
C	-5.294155000000	3.651936000000	-0.000008000000
C	-8.092913000000	3.631331000000	-0.000096000000
H	-7.946107000000	1.499191000000	-0.000042000000
C	-5.980435000000	4.847338000000	-0.000059000000
H	-4.210543000000	3.648102000000	0.000021000000
C	-7.398770000000	4.869967000000	-0.000102000000
H	-9.179083000000	3.632897000000	-0.000140000000
H	-5.436651000000	5.787703000000	-0.000068000000
C	-8.096340000000	-6.103435000000	0.000063000000
C	-8.103941000000	6.101206000000	-0.000145000000
N	-8.682889000000	7.117358000000	-0.000181000000
N	-8.670451000000	-7.117092000000	0.000096000000
N	2.459689000000	-0.001355000000	0.000062000000
C	3.127770000000	-0.000207000000	-1.220272000000
C	3.127843000000	-0.000896000000	1.220358000000
C	4.546628000000	0.000113000000	-1.263508000000
C	2.378212000000	0.000682000000	-2.426704000000
C	4.546702000000	-0.000600000000	1.263515000000
C	2.378346000000	-0.000628000000	2.426827000000
C	5.166985000000	0.000889000000	-2.512196000000
C	3.026239000000	0.001682000000	-3.645160000000
H	1.298315000000	0.000992000000	-2.386824000000
C	5.167124000000	-0.000538000000	2.512173000000
C	3.026436000000	-0.000292000000	3.645250000000
H	1.298446000000	-0.000223000000	2.386999000000
C	4.428731000000	0.001639000000	-3.693567000000

H	6.250674000000	0.001134000000	-2.557641000000
H	2.445701000000	0.002772000000	-4.561127000000
H	6.250815000000	-0.000333000000	2.557561000000
C	4.428931000000	-0.000405000000	3.693582000000
H	2.445947000000	0.000327000000	4.561247000000
H	4.942300000000	0.002493000000	-4.649138000000
H	4.942549000000	-0.000105000000	4.649127000000
C	5.393779000000	-0.000088000000	-0.000023000000
C	6.377813000000	-1.190807000000	-0.000449000000
C	6.377070000000	1.191260000000	0.000349000000
C	6.083635000000	-2.548514000000	-0.000904000000
C	7.708488000000	-0.734050000000	-0.000388000000
C	6.081945000000	2.548776000000	0.000747000000
C	7.708022000000	0.735369000000	0.000280000000
C	7.142452000000	-3.463526000000	-0.001392000000
H	5.055421000000	-2.900721000000	-0.000925000000
C	8.762528000000	-1.650802000000	-0.000965000000
C	7.140201000000	3.464416000000	0.001198000000
H	5.053556000000	2.900415000000	0.000744000000
C	8.761500000000	1.652770000000	0.000820000000
C	8.468483000000	-3.016198000000	-0.001457000000
H	6.931882000000	-4.528870000000	-0.001765000000
H	9.794707000000	-1.312035000000	-0.001105000000
C	8.466537000000	3.017958000000	0.001273000000
H	6.928900000000	4.529597000000	0.001529000000
H	9.793904000000	1.314681000000	0.000951000000
H	9.278920000000	-3.739315000000	-0.001893000000
H	9.276467000000	3.741634000000	0.001684000000

TZCN-DPA (T_1, Toluene)

E = -1675.50241319 Hartree

C	-2.983611000000	-1.133938000000	-0.133905000000
C	-1.008221000000	0.000000000000	-0.000001000000
C	-2.983611000000	1.133939000000	0.133904000000
N	-1.659491000000	1.191811000000	0.140771000000
N	-1.659492000000	-1.191811000000	-0.140773000000
N	-3.721383000000	0.000000000000	0.000000000000
C	0.438761000000	0.000000000000	-0.000002000000
C	1.177095000000	-1.214258000000	-0.131562000000
C	1.177095000000	1.214258000000	0.131559000000
C	2.554685000000	-1.216530000000	-0.125820000000
H	0.629295000000	-2.141674000000	-0.245422000000

C	2.554686000000	1.216530000000	0.125818000000
H	0.629295000000	2.141674000000	0.245419000000
C	3.270845000000	0.000000000000	-0.000001000000
H	3.099629000000	-2.147407000000	-0.249808000000
H	3.099629000000	2.147406000000	0.249806000000
C	-3.727019000000	-2.409883000000	-0.286353000000
C	-5.132832000000	-2.416337000000	-0.287994000000
C	-3.042461000000	-3.629360000000	-0.432210000000
C	-5.838294000000	-3.604684000000	-0.430581000000
H	-5.657634000000	-1.475301000000	-0.176176000000
C	-3.736156000000	-4.821948000000	-0.575311000000
H	-1.958794000000	-3.621687000000	-0.431226000000
C	-5.145025000000	-4.819142000000	-0.575541000000
H	-6.923699000000	-3.602367000000	-0.431036000000
H	-3.201387000000	-5.759711000000	-0.687583000000
C	-3.727019000000	2.409883000000	0.286353000000
C	-5.132832000000	2.416338000000	0.287995000000
C	-3.042460000000	3.629360000000	0.432209000000
C	-5.838293000000	3.604684000000	0.430582000000
H	-5.657634000000	1.475301000000	0.176178000000
C	-3.736155000000	4.821948000000	0.575311000000
H	-1.958793000000	3.621687000000	0.431224000000
C	-5.145024000000	4.819142000000	0.575541000000
H	-6.923699000000	3.602368000000	0.431038000000
H	-3.201385000000	5.759711000000	0.687582000000
C	-5.865667000000	-6.047161000000	-0.722746000000
C	-5.865666000000	6.047162000000	0.722747000000
N	-6.449708000000	7.047664000000	0.842540000000
N	-6.449710000000	-7.047663000000	-0.842539000000
N	4.690712000000	0.000000000000	0.000000000000
C	5.386588000000	0.954880000000	-0.767953000000
C	6.584702000000	1.524866000000	-0.286533000000
C	4.867463000000	1.364966000000	-2.014134000000
C	7.248462000000	2.478523000000	-1.047440000000
H	6.962696000000	1.239042000000	0.688743000000
C	5.546702000000	2.316648000000	-2.764166000000
H	3.956146000000	0.912534000000	-2.387569000000
C	6.736838000000	2.877826000000	-2.287812000000
H	8.161171000000	2.925317000000	-0.665517000000
H	5.151076000000	2.616070000000	-3.729637000000
H	7.260295000000	3.624257000000	-2.877007000000
C	5.386587000000	-0.954881000000	0.767953000000
C	6.584701000000	-1.524868000000	0.286534000000

C	4.867461000000	-1.364965000000	2.014134000000
C	7.248460000000	-2.478525000000	1.047442000000
H	6.962696000000	-1.239045000000	-0.688742000000
C	5.546700000000	-2.316648000000	2.764168000000
H	3.956144000000	-0.912533000000	2.387568000000
C	6.736836000000	-2.877827000000	2.287814000000
H	8.161170000000	-2.925319000000	0.665520000000
H	5.151073000000	-2.616068000000	3.729639000000
H	7.260292000000	-3.624257000000	2.877010000000

TZCN_DPAS (T_1, Toluene)

E = -2427.12114111 Hartree

C	5.409584000000	-1.132858000000	-0.004205000000
C	3.447072000000	0.005197000000	0.001550000000
C	5.420657000000	1.158637000000	0.006132000000
N	4.038919000000	1.182451000000	0.008854000000
N	4.043263000000	-1.204538000000	-0.006656000000
N	6.115772000000	-0.017422000000	0.001307000000
C	1.945792000000	0.004496000000	0.001893000000
C	1.236600000000	-1.202768000000	-0.037919000000
C	1.233309000000	1.210280000000	0.041671000000
C	-0.158362000000	-1.211627000000	-0.039057000000
H	1.793532000000	-2.131413000000	-0.068228000000
C	-0.159763000000	1.216878000000	0.041887000000
H	1.788907000000	2.140020000000	0.072274000000
C	-0.841694000000	0.000983000000	0.001122000000
H	-0.707927000000	-2.147810000000	-0.071416000000
H	-0.711173000000	2.151895000000	0.073991000000
C	6.150807000000	-2.418102000000	-0.007195000000
C	7.557483000000	-2.440262000000	-0.010712000000
C	5.455989000000	-3.640916000000	-0.005728000000
C	8.251366000000	-3.641074000000	-0.012683000000
H	8.091651000000	-1.497321000000	-0.011803000000
C	6.140033000000	-4.849633000000	-0.007496000000
H	4.372859000000	-3.622275000000	-0.002593000000
C	7.546230000000	-4.861300000000	-0.011013000000
H	9.336750000000	-3.648460000000	-0.015472000000
H	5.596140000000	-5.789153000000	-0.006039000000
C	6.140114000000	2.400437000000	0.007946000000
C	7.565535000000	2.436603000000	0.006656000000
C	5.455717000000	3.651317000000	0.010150000000
C	8.254471000000	3.629893000000	0.007546000000

H	8.107040000000	1.497791000000	0.004846000000
C	6.142330000000	4.846555000000	0.010934000000
H	4.372112000000	3.647635000000	0.010594000000
C	7.560658000000	4.868752000000	0.009662000000
H	9.340641000000	3.631178000000	0.006492000000
H	5.598817000000	5.787077000000	0.012386000000
C	8.254040000000	-6.104816000000	-0.012692000000
C	8.266230000000	6.099759000000	0.010176000000
N	8.845529000000	7.115715000000	0.010497000000
N	8.827802000000	-7.118692000000	-0.013941000000
N	-2.306973000000	0.000612000000	0.000621000000
C	-2.927270000000	-0.068135000000	1.260285000000
C	-2.926345000000	0.070954000000	-1.259362000000
C	-4.343888000000	-0.095881000000	1.434789000000
C	-2.086074000000	-0.111025000000	2.409536000000
C	-4.342879000000	0.097255000000	-1.434959000000
C	-2.084277000000	0.117392000000	-2.407868000000
C	-4.843643000000	-0.167425000000	2.736273000000
Si	-5.545694000000	0.000001000000	-0.000549000000
C	-2.625567000000	-0.183330000000	3.681762000000
H	-1.012756000000	-0.085192000000	2.301079000000
C	-4.841674000000	0.169980000000	-2.736733000000
C	-2.622835000000	0.191460000000	-3.680377000000
H	-1.010994000000	0.094020000000	-2.298551000000
C	-4.011205000000	-0.213817000000	3.859331000000
H	-5.919640000000	-0.185097000000	2.886684000000
H	-1.960151000000	-0.213898000000	4.537821000000
H	-5.917564000000	0.186537000000	-2.888013000000
C	-4.008382000000	0.219681000000	-3.859034000000
H	-1.956757000000	0.225717000000	-4.535776000000
H	-4.438830000000	-0.269938000000	4.854924000000
H	-4.435284000000	0.277210000000	-4.854856000000
C	-6.602402000000	-1.552957000000	-0.090029000000
C	-7.822509000000	-1.555493000000	-0.793949000000
C	-6.168894000000	-2.763207000000	0.483759000000
C	-8.578660000000	-2.721807000000	-0.919915000000
H	-8.196122000000	-0.637084000000	-1.240176000000
C	-6.923796000000	-3.930486000000	0.360837000000
H	-5.234938000000	-2.798199000000	1.039200000000
C	-8.129858000000	-3.911260000000	-0.342405000000
H	-9.518654000000	-2.700606000000	-1.464478000000
H	-6.571976000000	-4.852780000000	0.814896000000
H	-8.719009000000	-4.819156000000	-0.437880000000

C	-6.603973000000	1.551755000000	0.088200000000
C	-7.825142000000	1.552814000000	0.790274000000
C	-6.170299000000	2.762803000000	-0.483816000000
C	-8.582260000000	2.718513000000	0.916077000000
H	-8.198734000000	0.633800000000	1.235279000000
C	-6.926167000000	3.929458000000	-0.361002000000
H	-5.235409000000	2.799064000000	-1.037577000000
C	-8.133316000000	3.908767000000	0.340328000000
H	-9.523042000000	2.696253000000	1.459239000000
H	-6.574118000000	4.852415000000	-0.813486000000
H	-8.723133000000	4.816224000000	0.435792000000

TZCN-ICbz (T_1, Toluene)

E = -1959.53668527 Hartree

C	3.721784000000	1.124386000000	-0.331561000000
C	1.772175000000	-0.033845000000	-0.612366000000
C	3.729688000000	-1.150746000000	-0.235603000000
N	2.427652000000	-1.226961000000	-0.452388000000
N	2.419062000000	1.172948000000	-0.552688000000
N	4.458274000000	-0.005427000000	-0.158933000000
C	0.349054000000	-0.049103000000	-0.845189000000
C	-0.386404000000	1.158241000000	-1.017653000000
C	-0.377778000000	-1.272335000000	-0.904950000000
C	-1.755369000000	1.145564000000	-1.223600000000
H	0.149848000000	2.099324000000	-0.986636000000
C	-1.746729000000	-1.288727000000	-1.109373000000
H	0.165226000000	-2.202410000000	-0.785775000000
C	-2.447156000000	-0.078708000000	-1.264439000000
H	-2.301188000000	2.076905000000	-1.349556000000
H	-2.285889000000	-2.231649000000	-1.145748000000
C	4.452196000000	2.418889000000	-0.262645000000
C	5.838422000000	2.440348000000	-0.033886000000
C	3.773028000000	3.638785000000	-0.424061000000
C	6.530331000000	3.643614000000	0.034640000000
H	6.358610000000	1.497881000000	0.087547000000
C	4.452452000000	4.846581000000	-0.357701000000
H	2.704285000000	3.617826000000	-0.602807000000
C	5.841961000000	4.858631000000	-0.126164000000
H	7.601258000000	3.652328000000	0.211657000000
H	3.921440000000	5.784871000000	-0.483476000000
C	4.468569000000	-2.429809000000	-0.056360000000
C	5.847593000000	-2.421100000000	0.212770000000

C	3.804552000000	-3.664785000000	-0.152668000000
C	6.547380000000	-3.609582000000	0.383334000000
H	6.355518000000	-1.466991000000	0.285263000000
C	4.492179000000	-4.858137000000	0.014451000000
H	2.741255000000	-3.667172000000	-0.362506000000
C	5.874465000000	-4.839859000000	0.285359000000
H	7.612559000000	-3.595054000000	0.591822000000
H	3.973178000000	-5.808311000000	-0.062866000000
C	6.547705000000	6.102099000000	-0.054831000000
C	6.588700000000	-6.068189000000	0.460001000000
N	7.167323000000	-7.068894000000	0.602577000000
N	7.119408000000	7.115147000000	0.003925000000
N	-3.882748000000	-0.090548000000	-1.400676000000
C	-4.761355000000	-0.030047000000	-0.366732000000
C	-4.609677000000	-0.167880000000	-2.600234000000
C	-4.531740000000	0.058083000000	1.026047000000
C	-6.106611000000	-0.066326000000	-0.854507000000
C	-4.119205000000	-0.245820000000	-3.901597000000
C	-5.994331000000	-0.155683000000	-2.303635000000
C	-5.646393000000	0.109088000000	1.923134000000
N	-3.379562000000	0.109884000000	1.741427000000
C	-7.173421000000	-0.016518000000	0.030363000000
C	-5.060086000000	-0.313196000000	-4.930275000000
H	-3.053175000000	-0.253092000000	-4.099633000000
C	-6.916353000000	-0.223791000000	-3.347876000000
C	-6.942348000000	0.072062000000	1.428846000000
C	-5.076362000000	0.197573000000	3.261630000000
C	-3.668236000000	0.196162000000	3.103908000000
H	-2.451191000000	0.090958000000	1.335176000000
H	-8.194354000000	-0.044189000000	-0.335974000000
C	-6.437082000000	-0.302366000000	-4.659108000000
H	-4.718061000000	-0.374756000000	-5.958582000000
H	-7.984527000000	-0.215895000000	-3.152095000000
H	-7.790511000000	0.110792000000	2.104236000000
C	-5.615439000000	0.276809000000	4.545328000000
C	-2.787136000000	0.272484000000	4.180270000000
H	-7.142973000000	-0.355895000000	-5.482079000000
C	-4.742187000000	0.353128000000	5.634842000000
H	-6.690015000000	0.279622000000	4.700838000000
C	-3.350502000000	0.351210000000	5.454626000000
H	-1.712054000000	0.271346000000	4.033967000000
H	-5.148645000000	0.415256000000	6.639362000000
H	-2.698468000000	0.412171000000	6.319958000000

TZCN-DPAC (T_1, Toluene)

E = -2175.70081823 Hartree

C	-5.025566000000	1.162339000000	0.001271000000
C	-3.159378000000	-0.127457000000	0.009819000000
C	-5.218161000000	-1.120841000000	0.005062000000
N	-3.842898000000	-1.254057000000	0.011601000000
N	-3.658319000000	1.125859000000	0.003444000000
N	-5.818183000000	0.106769000000	0.001444000000
C	-1.662926000000	-0.245218000000	0.014776000000
C	-0.861292000000	0.902383000000	-0.024876000000
C	-1.048303000000	-1.503888000000	0.059013000000
C	0.530032000000	0.802175000000	-0.022723000000
H	-1.343564000000	1.871810000000	-0.057961000000
C	0.339536000000	-1.620490000000	0.063302000000
H	-1.675547000000	-2.386886000000	0.090132000000
C	1.115432000000	-0.460595000000	0.020983000000
H	1.152514000000	1.691299000000	-0.054475000000
H	0.815084000000	-2.596309000000	0.099046000000
C	-5.663069000000	2.502421000000	-0.000515000000
C	-7.063520000000	2.634836000000	-0.005588000000
C	-4.874137000000	3.666526000000	0.003769000000
C	-7.660861000000	3.886557000000	-0.006314000000
H	-7.669878000000	1.736599000000	-0.008767000000
C	-5.460991000000	4.925379000000	0.003164000000
H	-3.795833000000	3.562611000000	0.008098000000
C	-6.861898000000	5.047427000000	-0.001870000000
H	-8.742278000000	3.979307000000	-0.010167000000
H	-4.844857000000	5.819183000000	0.006729000000
C	-6.034401000000	-2.300917000000	0.001339000000
C	-7.458074000000	-2.221480000000	-0.004049000000
C	-5.453321000000	-3.602926000000	0.001982000000
C	-8.241190000000	-3.355117000000	-0.008506000000
H	-7.920871000000	-1.241368000000	-0.004620000000
C	-6.234291000000	-4.738712000000	-0.002556000000
H	-4.372911000000	-3.686433000000	0.005513000000
C	-7.649895000000	-4.646096000000	-0.007941000000
H	-9.323872000000	-3.268717000000	-0.012566000000
H	-5.768353000000	-5.719970000000	-0.002203000000
C	-7.469873000000	6.342765000000	-0.002252000000
C	-8.453127000000	-5.815610000000	-0.012835000000
N	-9.113090000000	-6.781145000000	-0.016909000000

N	-7.962051000000	7.398638000000	-0.002466000000
N	2.570866000000	-0.555186000000	0.024082000000
C	3.244406000000	-0.592390000000	1.240353000000
C	3.243601000000	-0.710671000000	-1.181977000000
C	4.664112000000	-0.511722000000	1.266630000000
C	2.512460000000	-0.763408000000	2.441646000000
C	4.664536000000	-0.640110000000	-1.214398000000
C	2.511708000000	-0.994436000000	-2.362249000000
C	5.303354000000	-0.680190000000	2.490993000000
C	3.181009000000	-0.909658000000	3.643525000000
H	1.432691000000	-0.804805000000	2.411581000000
C	5.303513000000	-0.942046000000	-2.412887000000
C	3.180453000000	-1.268655000000	-3.541119000000
H	1.431585000000	-1.022237000000	-2.330654000000
C	4.580483000000	-0.886471000000	3.670680000000
H	6.385265000000	-0.634564000000	2.530092000000
H	2.615448000000	-1.054466000000	4.557425000000
H	6.385963000000	-0.913800000000	-2.453696000000
C	4.580297000000	-1.263493000000	-3.566379000000
H	2.615085000000	-1.500090000000	-4.437098000000
H	5.110922000000	-1.016728000000	4.608131000000
H	5.110898000000	-1.496785000000	-4.483539000000
C	5.425111000000	-0.107392000000	0.002388000000
C	6.866179000000	-0.666235000000	0.035602000000
C	7.997184000000	0.155340000000	0.019620000000
C	7.049907000000	-2.058796000000	0.092873000000
C	9.281376000000	-0.399580000000	0.057278000000
H	7.887082000000	1.232831000000	-0.022002000000
C	8.327414000000	-2.611718000000	0.129638000000
H	6.184380000000	-2.716113000000	0.108965000000
C	9.451830000000	-1.780967000000	0.111543000000
H	10.146076000000	0.257840000000	0.043732000000
H	8.445067000000	-3.690840000000	0.172828000000
H	10.449282000000	-2.210029000000	0.140159000000
C	5.407196000000	1.464456000000	-0.086535000000
C	5.495812000000	2.115575000000	-1.327207000000
C	5.355099000000	2.258742000000	1.069166000000
C	5.534274000000	3.507955000000	-1.408750000000
H	5.538409000000	1.543744000000	-2.246470000000
C	5.391909000000	3.652032000000	0.987410000000
H	5.287943000000	1.801327000000	2.048758000000
C	5.478715000000	4.284965000000	-0.251716000000
H	5.603475000000	3.981896000000	-2.383744000000

H	5.348902000000	4.239118000000	1.900374000000
H	5.501614000000	5.368881000000	-0.315448000000

TZCN-SSiAS (T_1, Toluene)

E = -2425.92935473 Hartree

C	-5.512834000000	1.144921000000	-0.000839000000
C	-3.543276000000	-0.000188000000	0.000076000000
C	-5.513467000000	-1.144319000000	0.000872000000
N	-4.131264000000	-1.193455000000	0.001881000000
N	-4.130654000000	1.193475000000	-0.001772000000
N	-6.206071000000	0.000574000000	0.000008000000
C	-2.038241000000	-0.000580000000	0.000121000000
C	-1.328716000000	1.206119000000	-0.015416000000
C	-1.329346000000	-1.207653000000	0.015692000000
C	0.065726000000	1.213856000000	-0.015853000000
H	-1.885956000000	2.135118000000	-0.027175000000
C	0.065084000000	-1.216123000000	0.016165000000
H	-1.887077000000	-2.136356000000	0.027437000000
C	0.747123000000	-0.001307000000	0.000164000000
H	0.616701000000	2.149605000000	-0.028236000000
H	0.615563000000	-2.152164000000	0.028556000000
C	-6.245045000000	2.404679000000	-0.000545000000
C	-7.661112000000	2.434830000000	-0.001097000000
C	-5.555514000000	3.641681000000	0.000650000000
C	-8.352212000000	3.631578000000	-0.000559000000
H	-8.200075000000	1.494476000000	-0.001968000000
C	-6.241003000000	4.843951000000	0.001267000000
H	-4.472210000000	3.630571000000	0.001368000000
C	-7.652442000000	4.861572000000	0.000638000000
H	-9.437979000000	3.635905000000	-0.001043000000
H	-5.696861000000	5.783767000000	0.002311000000
C	-6.246279000000	-2.403563000000	0.000521000000
C	-7.662420000000	-2.432991000000	0.001015000000
C	-5.557445000000	-3.641022000000	-0.000687000000
C	-8.354152000000	-3.629343000000	0.000412000000
H	-8.200894000000	-1.492357000000	0.001890000000
C	-6.243592000000	-4.842881000000	-0.001369000000
H	-4.474133000000	-3.630545000000	-0.001366000000
C	-7.655079000000	-4.859771000000	-0.000795000000
H	-9.439922000000	-3.633060000000	0.000850000000
H	-5.699957000000	-5.782994000000	-0.002424000000
C	-8.358770000000	6.098982000000	0.001276000000

C	-8.362070000000	-6.096762000000	-0.001502000000
N	-8.939125000000	-7.111362000000	-0.002098000000
N	-8.935259000000	7.113887000000	0.001816000000
N	2.212685000000	-0.001636000000	0.000146000000
C	2.832297000000	0.021395000000	1.261674000000
C	2.832212000000	-0.025055000000	-1.261411000000
C	4.249160000000	0.026267000000	1.437747000000
C	1.992842000000	0.039966000000	2.412675000000
C	4.249063000000	-0.029532000000	-1.437591000000
C	1.992670000000	-0.044529000000	-2.412331000000
C	4.753611000000	0.049688000000	2.739099000000
C	2.535470000000	0.063041000000	3.685594000000
H	0.919071000000	0.035868000000	2.305134000000
C	4.753416000000	-0.053777000000	-2.738967000000
C	2.535202000000	-0.068360000000	-3.685277000000
H	0.918906000000	-0.040635000000	-2.304705000000
C	3.921778000000	0.068359000000	3.863203000000
H	5.830295000000	0.053262000000	2.885180000000
H	1.871393000000	0.076746000000	4.543116000000
H	5.830089000000	-0.057127000000	-2.885134000000
C	3.921498000000	-0.073513000000	-3.862990000000
H	1.871061000000	-0.082815000000	-4.542736000000
H	4.349919000000	0.086409000000	4.859930000000
H	4.349565000000	-0.092201000000	-4.859737000000
C	6.733056000000	1.352221000000	-0.028808000000
C	6.735536000000	-1.350957000000	0.028684000000
C	6.618839000000	2.743439000000	-0.060053000000
C	8.016651000000	0.746724000000	-0.017518000000
C	6.623865000000	-2.742387000000	0.059894000000
C	8.018022000000	-0.743116000000	0.017276000000
C	7.765760000000	3.543087000000	-0.080647000000
H	5.638828000000	3.215057000000	-0.068888000000
C	9.158421000000	1.554507000000	-0.040037000000
C	7.772252000000	-3.539931000000	0.080341000000
H	5.644726000000	-3.215821000000	0.068806000000
C	9.161279000000	-1.548805000000	0.039655000000
C	9.027894000000	2.944845000000	-0.071092000000
H	7.675754000000	4.625254000000	-0.104742000000
H	10.150360000000	1.112042000000	-0.034713000000
C	9.033291000000	-2.939380000000	0.070683000000
H	7.684232000000	-4.622262000000	0.104407000000
H	10.152415000000	-1.104532000000	0.034238000000
H	9.919887000000	3.564979000000	-0.088278000000

H	9.926415000000	-3.557886000000	0.087758000000
Si	5.438835000000	-0.000562000000	0.000018000000

TZCN-Cbz (T_1, Toluene)

E = -1674.32354198 Hartree

C	3.063762000000	-1.135914000000	0.111174000000
C	1.086766000000	0.000000000000	-0.000001000000
C	3.063762000000	1.135914000000	-0.111175000000
N	1.740854000000	1.195365000000	-0.117098000000
N	1.740854000000	-1.195365000000	0.117097000000
N	3.802093000000	0.000000000000	-0.000001000000
C	-0.355858000000	0.000000000000	0.000000000000
C	-1.096176000000	-1.216772000000	0.109808000000
C	-1.096176000000	1.216772000000	-0.109809000000
C	-2.474031000000	-1.219418000000	0.101094000000
H	-0.548805000000	-2.146011000000	0.210376000000
C	-2.474031000000	1.219418000000	-0.101094000000
H	-0.548805000000	2.146011000000	-0.210377000000
C	-3.185051000000	0.000000000000	0.000000000000
H	-3.019731000000	-2.150833000000	0.219533000000
H	-3.019732000000	2.150833000000	-0.219533000000
C	3.809170000000	-2.415012000000	0.238320000000
C	5.214526000000	-2.420580000000	0.238937000000
C	3.125227000000	-3.636972000000	0.360925000000
C	5.920888000000	-3.611260000000	0.357665000000
H	5.738734000000	-1.477209000000	0.145520000000
C	3.819614000000	-4.832039000000	0.480154000000
H	2.041566000000	-3.629298000000	0.361163000000
C	5.228168000000	-4.828371000000	0.479208000000
H	7.006273000000	-3.608452000000	0.357396000000
H	3.285408000000	-5.772079000000	0.574604000000
C	3.809170000000	2.415012000000	-0.238321000000
C	5.214526000000	2.420580000000	-0.238937000000
C	3.125228000000	3.636972000000	-0.360926000000
C	5.920888000000	3.611260000000	-0.357664000000
H	5.738734000000	1.477209000000	-0.145520000000
C	3.819614000000	4.832039000000	-0.480155000000
H	2.041566000000	3.629298000000	-0.361165000000
C	5.228168000000	4.828371000000	-0.479208000000
H	7.006273000000	3.608452000000	-0.357395000000
H	3.285409000000	5.772079000000	-0.574604000000
C	5.949595000000	-6.058961000000	0.601571000000

C	5.949595000000	6.058961000000	-0.601569000000
N	6.534193000000	7.061254000000	-0.701092000000
N	6.534193000000	-7.061254000000	0.701094000000
N	-4.603490000000	0.000000000000	0.000000000000
C	-5.416358000000	-0.771189000000	-0.830154000000
C	-5.416358000000	0.771190000000	0.830154000000
C	-5.037694000000	-1.648979000000	-1.853728000000
C	-6.778109000000	-0.497854000000	-0.532777000000
C	-5.037693000000	1.648979000000	1.853728000000
C	-6.778109000000	0.497855000000	0.532778000000
C	-6.057708000000	-2.289924000000	-2.557356000000
H	-3.995040000000	-1.814996000000	-2.096311000000
C	-7.776115000000	-1.138544000000	-1.252027000000
C	-6.057708000000	2.289924000000	2.557356000000
H	-3.995040000000	1.814996000000	2.096311000000
C	-7.776115000000	1.138544000000	1.252027000000
C	-7.405265000000	-2.044560000000	-2.261063000000
H	-5.800414000000	-2.980765000000	-3.353370000000
H	-8.824622000000	-0.941555000000	-1.051001000000
C	-7.405265000000	2.044560000000	2.261064000000
H	-5.800414000000	2.980765000000	3.353370000000
H	-8.824622000000	0.941555000000	1.051002000000
H	-8.178338000000	-2.552721000000	-2.828530000000
H	-8.178337000000	2.552721000000	2.828531000000

Table S12. Optimized Cartesian coordinates of donor units (Figure 2) in the gas phase.

All geometries were optimized at the B3LYP/6-31G(d) level of theory.

PXZ (S_0, Gas Phase)		
E = -592.668196893 Hartree		
C	1.208632000000	0.727447000000	0.095025000000
C	-1.208632000000	0.727447000000	0.095025000000
C	2.434957000000	1.379890000000	-0.042809000000
C	1.185643000000	-0.678292000000	0.095152000000
C	-1.185643000000	-0.678292000000	0.095153000000
C	-2.434957000000	1.379890000000	-0.042808000000
C	3.618854000000	0.646489000000	-0.167651000000
H	2.459215000000	2.467441000000	-0.043933000000
C	2.357544000000	-1.408283000000	-0.036286000000
C	-2.357544000000	-1.408283000000	-0.036286000000
H	-2.459215000000	2.467441000000	-0.043933000000
C	-3.618854000000	0.646489000000	-0.167652000000
C	3.583924000000	-0.745590000000	-0.163263000000
H	4.563754000000	1.172451000000	-0.268187000000
H	2.294278000000	-2.491954000000	-0.033778000000
C	-3.583924000000	-0.745590000000	-0.163263000000
H	-2.294278000000	-2.491954000000	-0.033778000000
H	-4.563754000000	1.172451000000	-0.268187000000
H	4.499273000000	-1.321451000000	-0.259312000000
H	-4.499273000000	-1.321450000000	-0.259313000000
N	0.000000000000	1.414536000000	0.256409000000
O	0.000000000000	-1.377110000000	0.251349000000
H	0.000000000000	2.402226000000	0.042750000000
DMAC (S_0, Gas Phase)		
E = -635.399293422 Hartree		
N	0.000033000000	-1.687425000000	0.000302000000
C	1.223408000000	-1.034449000000	-0.000114000000
C	-1.223355000000	-1.034468000000	0.000275000000
C	1.273957000000	0.373478000000	-0.000259000000
C	2.407057000000	-1.792262000000	-0.000230000000
C	-1.273944000000	0.373458000000	0.000169000000
C	-2.406988000000	-1.792306000000	0.000215000000
C	2.540176000000	0.971737000000	-0.000146000000
C	3.646856000000	-1.165832000000	-0.000313000000
H	2.340274000000	-2.878600000000	-0.000172000000

C	-2.540171000000	0.971691000000	-0.000299000000
C	-3.646801000000	-1.165903000000	-0.000060000000
H	-2.340180000000	-2.878643000000	0.000307000000
C	3.719754000000	0.228277000000	-0.000197000000
H	2.608954000000	2.056193000000	0.000046000000
H	4.552681000000	-1.766205000000	-0.000343000000
H	-2.608970000000	2.056147000000	-0.000623000000
C	-3.719733000000	0.228205000000	-0.000387000000
H	-4.552612000000	-1.766297000000	-0.000152000000
H	4.681723000000	0.732249000000	-0.000115000000
H	-4.681713000000	0.732154000000	-0.000732000000
C	-0.000034000000	1.237895000000	0.000129000000
C	-0.000427000000	2.137082000000	-1.265240000000
H	-0.884946000000	2.782635000000	-1.289526000000
H	0.883630000000	2.783244000000	-1.289699000000
H	-0.000315000000	1.526785000000	-2.174188000000
C	0.000265000000	2.136481000000	1.265942000000
H	0.884725000000	2.782109000000	1.290509000000
H	-0.883899000000	2.782494000000	1.290714000000
H	0.000246000000	1.525744000000	2.174595000000
H	0.000042000000	-2.696535000000	0.000352000000

TPA (S_0, Gas Phase)

E = -749.697345315 Hartree

C	-4.235700000000	0.036419000000	0.000074000000
C	-3.521180000000	0.937728000000	-0.791956000000
C	-3.536702000000	-0.877035000000	0.792038000000
C	-2.127748000000	0.923430000000	-0.802573000000
H	-4.050187000000	1.650167000000	-1.419744000000
C	-2.143230000000	-0.886702000000	0.802491000000
H	-4.077813000000	-1.580270000000	1.419887000000
C	-1.421775000000	0.012217000000	-0.000092000000
H	-1.578136000000	1.616947000000	-1.431014000000
H	-1.605563000000	-1.589568000000	1.430871000000
N	-0.000200000000	-0.000017000000	-0.000186000000
C	0.700174000000	-1.237212000000	-0.000092000000
C	0.265336000000	-2.303675000000	-0.803971000000
C	1.838297000000	-1.412880000000	0.803939000000
C	0.949846000000	-3.517476000000	-0.793245000000
H	-0.609259000000	-2.174140000000	-1.433481000000
C	2.526873000000	-2.624377000000	0.793621000000
H	2.177168000000	-0.596149000000	1.433297000000

C	2.086554000000	-3.685969000000	0.000305000000
H	0.598393000000	-4.331468000000	-1.422081000000
H	3.405603000000	-2.741689000000	1.422595000000
H	2.621721000000	-4.631265000000	0.000472000000
C	0.721279000000	1.224988000000	-0.000159000000
C	0.305033000000	2.298439000000	0.804251000000
C	1.861982000000	1.381398000000	-0.804498000000
C	1.010287000000	3.500304000000	0.793821000000
H	-0.571431000000	2.183648000000	1.434018000000
C	2.571289000000	2.580878000000	-0.793874000000
H	2.186487000000	0.559227000000	-1.434350000000
C	2.149508000000	3.649546000000	0.000019000000
H	0.673060000000	4.319957000000	1.423094000000
H	3.451707000000	2.683350000000	-1.423079000000
H	2.700850000000	4.585500000000	0.000083000000
H	-5.321934000000	0.045760000000	0.000130000000

PTZ (S_0, Gas Phase)

E = -915.643610053 Hartree

C	0.746910000000	-0.242548000000	1.230469000000
C	0.746910000000	-0.242548000000	-1.230469000000
C	1.567329000000	-0.014128000000	2.341953000000
C	-0.644359000000	-0.087242000000	1.364873000000
C	-0.644359000000	-0.087242000000	-1.364873000000
C	1.567329000000	-0.014128000000	-2.341953000000
C	1.013797000000	0.344143000000	3.570817000000
H	2.644949000000	-0.125846000000	2.239515000000
C	-1.187230000000	0.310557000000	2.586994000000
C	-1.187230000000	0.310557000000	-2.586994000000
H	2.644949000000	-0.125846000000	-2.239515000000
C	1.013797000000	0.344143000000	-3.570817000000
C	-0.364562000000	0.513804000000	3.697131000000
H	1.666829000000	0.503025000000	4.424312000000
H	-2.262152000000	0.445676000000	2.669095000000
C	-0.364562000000	0.513804000000	-3.697131000000
H	-2.262152000000	0.445676000000	-2.669095000000
H	1.666829000000	0.503025000000	-4.424312000000
H	-0.800297000000	0.804549000000	4.648252000000
H	-0.800297000000	0.804549000000	-4.648252000000
N	1.301589000000	-0.630892000000	0.000000000000
S	-1.719076000000	-0.503654000000	0.000000000000
H	2.312807000000	-0.675144000000	0.000000000000

SAF (S_0, Gas Phase)

E = -1017.67973581 Hartree

N	-2.934482000000	-0.000001000000	0.181379000000
C	-2.300265000000	-1.219888000000	-0.031347000000
C	-2.300265000000	1.219888000000	-0.031339000000
C	-0.903961000000	-1.270804000000	-0.195175000000
C	-3.062054000000	-2.400127000000	-0.076216000000
C	-0.903961000000	1.270805000000	-0.195167000000
C	-3.062055000000	2.400127000000	-0.076203000000
C	-0.309866000000	-2.521804000000	-0.400674000000
C	-2.445852000000	-3.628366000000	-0.278166000000
H	-4.141697000000	-2.339738000000	0.047154000000
C	-0.309866000000	2.521806000000	-0.400661000000
C	-2.445853000000	3.628368000000	-0.278146000000
H	-4.141697000000	2.339737000000	0.047167000000
C	-1.059724000000	-3.694637000000	-0.443544000000
H	0.767604000000	-2.571724000000	-0.527331000000
H	-3.048316000000	-4.532206000000	-0.310782000000
H	0.767603000000	2.571726000000	-0.527317000000
C	-1.059724000000	3.694639000000	-0.443524000000
H	-3.048316000000	4.532207000000	-0.310757000000
H	-0.567621000000	-4.649580000000	-0.602109000000
H	-0.567621000000	4.649583000000	-0.602085000000
C	-0.045091000000	0.000000000000	-0.079677000000
C	0.746103000000	-0.000004000000	1.244371000000
C	1.103757000000	0.000004000000	-1.097786000000
C	0.255904000000	-0.000008000000	2.544528000000
C	2.132298000000	-0.000004000000	1.001169000000
C	1.023980000000	0.000010000000	-2.485394000000
C	2.354110000000	0.000002000000	-0.451814000000
C	1.163257000000	-0.000012000000	3.609665000000
H	-0.814325000000	-0.000009000000	2.733744000000
C	3.037051000000	-0.000008000000	2.064914000000
C	2.206829000000	0.000012000000	-3.232450000000
H	0.057427000000	0.000012000000	-2.982340000000
C	3.535027000000	0.000004000000	-1.198580000000
C	2.542066000000	-0.000012000000	3.370818000000
H	0.793580000000	-0.000015000000	4.631623000000
H	4.109157000000	-0.000008000000	1.884344000000
C	3.451639000000	0.000009000000	-2.592535000000
H	2.158605000000	0.000016000000	-4.318092000000

H	4.504540000000	0.000002000000	-0.706829000000
H	3.234017000000	-0.000015000000	4.208894000000
H	4.362144000000	0.000011000000	-3.186019000000
H	-3.944623000000	-0.000001000000	0.168671000000

DPA (S_0, Gas Phase)

E = -518.651797211 Hartree

N	0.000000000000	1.033655000000	0.000003000000
C	-1.266939000000	0.440042000000	-0.019131000000
C	-1.499895000000	-0.852764000000	-0.521016000000
C	-2.364926000000	1.193963000000	0.434195000000
C	-2.793243000000	-1.372405000000	-0.542584000000
H	-0.675983000000	-1.436085000000	-0.916080000000
C	-3.653523000000	0.669590000000	0.391665000000
H	-2.196761000000	2.194542000000	0.827345000000
C	-3.879290000000	-0.622317000000	-0.088406000000
H	-2.951124000000	-2.373523000000	-0.935917000000
H	-4.484598000000	1.273658000000	0.746689000000
H	-4.883555000000	-1.034886000000	-0.111865000000
C	1.266939000000	0.440042000000	0.019133000000
C	1.499897000000	-0.852763000000	0.521019000000
C	2.364924000000	1.193963000000	-0.434196000000
C	2.793245000000	-1.372404000000	0.542584000000
H	0.675985000000	-1.436084000000	0.916086000000
C	3.653522000000	0.669591000000	-0.391669000000
H	2.196759000000	2.194541000000	-0.827347000000
C	3.879291000000	-0.622317000000	0.088403000000
H	2.951126000000	-2.373522000000	0.935918000000
H	4.484596000000	1.273658000000	-0.746696000000
H	4.883555000000	-1.034885000000	0.111860000000
H	0.000000000000	2.043675000000	0.000005000000

DPAS (S_0, Gas Phase)

E = -1270.28823604 Hartree

N	-2.975512000000	-0.000914000000	-0.000011000000
C	-2.387492000000	0.686672000000	1.057896000000
C	-2.387090000000	-0.689709000000	-1.056910000000
C	-0.986117000000	0.799771000000	1.220518000000
C	-3.255842000000	1.287421000000	1.993702000000
C	-0.985651000000	-0.802727000000	-1.219059000000
C	-3.255101000000	-1.291790000000	-1.992173000000

C	-0.515584000000	1.517031000000	2.337432000000
Si	0.188693000000	-0.000094000000	0.000047000000
C	-2.751718000000	1.988606000000	3.078567000000
H	-4.332385000000	1.195502000000	1.858901000000
C	-0.514727000000	-1.521609000000	-2.334767000000
C	-2.750591000000	-1.994374000000	-3.075952000000
H	-4.331693000000	-1.199887000000	-1.857754000000
C	-1.369372000000	2.109641000000	3.261526000000
H	0.558934000000	1.609881000000	2.482669000000
H	-3.440258000000	2.442355000000	3.786835000000
H	0.559841000000	-1.614670000000	-2.479500000000
C	-1.368180000000	-2.115605000000	-3.258280000000
H	-3.438877000000	-2.449161000000	-3.783801000000
H	-0.970689000000	2.655813000000	4.111350000000
H	-0.969189000000	-2.662972000000	-4.107190000000
C	1.291082000000	1.301229000000	-0.822143000000
C	2.501670000000	0.950769000000	-1.449990000000
C	0.890569000000	2.648599000000	-0.886555000000
C	3.276305000000	1.901794000000	-2.116313000000
H	2.853408000000	-0.077741000000	-1.409709000000
C	1.662580000000	3.604906000000	-1.548336000000
H	-0.035651000000	2.956387000000	-0.407303000000
C	2.857519000000	3.232590000000	-2.166430000000
H	4.207752000000	1.605183000000	-2.592353000000
H	1.332265000000	4.640284000000	-1.580371000000
H	3.460530000000	3.975698000000	-2.682249000000
C	1.295264000000	-1.298654000000	0.820909000000
C	2.506688000000	-0.945499000000	1.445617000000
C	0.897195000000	-2.646646000000	0.887587000000
C	3.284473000000	-1.894543000000	2.111109000000
H	2.856567000000	0.083566000000	1.403480000000
C	1.672357000000	-3.600969000000	1.548532000000
H	-0.029597000000	-2.956496000000	0.410773000000
C	2.868082000000	-3.225995000000	2.163507000000
H	4.216505000000	-1.595868000000	2.584709000000
H	1.343890000000	-4.636878000000	1.582355000000
H	3.473545000000	-3.967562000000	2.678672000000
H	-3.985928000000	-0.001165000000	-0.000041000000

ICbz (S_0, Gas Phase)

E = -802.687427094 Hartree

N	1.616125000000	-1.437900000000	-0.027420000000

C	0.698421000000	-0.392554000000	-0.001770000000
C	2.901135000000	-0.909536000000	-0.003012000000
C	-0.698423000000	-0.392555000000	0.001798000000
C	1.395056000000	0.839708000000	-0.013531000000
C	4.131476000000	-1.568877000000	0.017987000000
C	2.806176000000	0.507684000000	-0.016761000000
C	-1.395056000000	0.839706000000	0.013556000000
N	-1.616124000000	-1.437912000000	0.027503000000
C	0.692681000000	2.063723000000	-0.010041000000
C	5.284328000000	-0.786622000000	0.019097000000
H	4.190460000000	-2.654165000000	0.031031000000
C	3.982454000000	1.268594000000	-0.022279000000
C	-0.692682000000	2.063723000000	0.010082000000
C	-2.806177000000	0.507683000000	0.016761000000
C	-2.901135000000	-0.909536000000	0.003030000000
H	-1.402592000000	-2.401909000000	-0.175350000000
H	1.239805000000	3.002105000000	-0.017437000000
C	5.212716000000	0.617636000000	-0.003609000000
H	6.255864000000	-1.272974000000	0.035665000000
H	3.934719000000	2.354331000000	-0.036726000000
H	-1.239806000000	3.002105000000	0.017482000000
C	-3.982454000000	1.268594000000	0.022247000000
C	-4.131475000000	-1.568875000000	-0.017996000000
H	6.130108000000	1.199441000000	-0.005485000000
C	-5.212716000000	0.617637000000	0.003550000000
H	-3.934718000000	2.354332000000	0.036691000000
C	-5.284328000000	-0.786621000000	-0.019149000000
H	-4.190458000000	-2.654164000000	-0.031028000000
H	-6.130107000000	1.199442000000	0.005401000000
H	-6.255864000000	-1.272973000000	-0.035741000000
H	1.402583000000	-2.401949000000	0.175157000000

DPAC (S_0, Gas Phase)

E = -1018.86294087 Hartree

N	2.637351000000	0.000881000000	0.481742000000
C	1.972627000000	-1.207555000000	0.696293000000
C	1.971893000000	1.208986000000	0.695933000000
C	0.569984000000	-1.248076000000	0.571417000000
C	2.691764000000	-2.358685000000	1.048501000000
C	0.569228000000	1.248595000000	0.571007000000
C	2.690328000000	2.360677000000	1.047735000000
C	-0.077600000000	-2.458179000000	0.844116000000

C	2.024235000000	-3.554747000000	1.290315000000
H	3.774579000000	-2.303774000000	1.142271000000
C	-0.079111000000	2.458339000000	0.843460000000
C	2.022056000000	3.556391000000	1.289228000000
H	3.773182000000	2.306471000000	1.141462000000
C	0.632137000000	-3.606278000000	1.199404000000
H	-1.158674000000	-2.504583000000	0.762584000000
H	2.591431000000	-4.440523000000	1.563501000000
H	-1.160231000000	2.504012000000	0.762178000000
C	0.629919000000	3.606990000000	1.198420000000
H	2.588704000000	4.442614000000	1.562102000000
H	0.100807000000	-4.533028000000	1.395179000000
H	0.098002000000	4.533443000000	1.394011000000
C	-0.160172000000	-0.000024000000	0.032298000000
C	-1.632900000000	-0.000339000000	0.506285000000
C	-2.719636000000	-0.001011000000	-0.374127000000
C	-1.901602000000	-0.000129000000	1.886744000000
C	-4.034148000000	-0.001412000000	0.106410000000
H	-2.548245000000	-0.001234000000	-1.444467000000
C	-3.208112000000	-0.000514000000	2.367424000000
H	-1.072383000000	0.000343000000	2.588365000000
C	-4.285136000000	-0.001152000000	1.475935000000
H	-4.859858000000	-0.001929000000	-0.600593000000
H	-3.386303000000	-0.000324000000	3.439780000000
H	-5.306083000000	-0.001454000000	1.848586000000
C	-0.071168000000	-0.000263000000	-1.528384000000
C	-0.056680000000	1.200327000000	-2.253620000000
C	-0.054579000000	-1.201044000000	-2.253263000000
C	-0.026747000000	1.201580000000	-3.649180000000
H	-0.062593000000	2.148464000000	-1.727565000000
C	-0.024627000000	-1.202657000000	-3.648827000000
H	-0.058779000000	-2.149022000000	-1.726905000000
C	-0.008907000000	-0.000630000000	-4.355939000000
H	-0.012300000000	2.149117000000	-4.182007000000
H	-0.008467000000	-2.150319000000	-4.181384000000
H	0.019691000000	-0.000768000000	-5.442441000000
H	3.627783000000	0.001193000000	0.687639000000

SSiAS (S_0, Gas Phase)

E = -1269.09505244 Hartree

N	-3.211160000000	0.000010000000	0.000844000000
C	-2.622262000000	-1.261224000000	0.000379000000

C	-2.622252000000	1.261239000000	0.000090000000
C	-1.220600000000	-1.457992000000	-0.000186000000
C	-3.487922000000	-2.375501000000	0.000407000000
C	-1.220588000000	1.457996000000	-0.000519000000
C	-3.487902000000	2.375522000000	0.000065000000
C	-0.744163000000	-2.783520000000	-0.000808000000
C	-2.979482000000	-3.665346000000	-0.000157000000
H	-4.564895000000	-2.215412000000	0.000845000000
C	-0.744141000000	2.783520000000	-0.001200000000
C	-2.979453000000	3.665364000000	-0.000597000000
H	-4.564877000000	2.215442000000	0.000553000000
C	-1.596047000000	-3.881879000000	-0.000794000000
H	0.331113000000	-2.949898000000	-0.001337000000
H	-3.665623000000	-4.508451000000	-0.000125000000
H	0.331137000000	2.949889000000	-0.001674000000
C	-1.596016000000	3.881885000000	-0.001255000000
H	-3.665587000000	4.508474000000	-0.000622000000
H	-1.195982000000	-4.891498000000	-0.001284000000
H	-1.195942000000	4.891501000000	-0.001770000000
C	1.265692000000	0.000719000000	1.344773000000
C	1.266202000000	-0.000732000000	-1.344532000000
C	1.156391000000	0.000627000000	2.736577000000
C	2.550718000000	0.000141000000	0.745453000000
C	1.157428000000	-0.000641000000	-2.736379000000
C	2.551001000000	-0.000151000000	-0.744721000000
C	2.301555000000	0.000289000000	3.539040000000
H	0.174838000000	0.000947000000	3.206157000000
C	3.693650000000	-0.000209000000	1.552861000000
C	2.302895000000	-0.000302000000	-3.538407000000
H	0.176053000000	-0.000963000000	-3.206328000000
C	3.694238000000	0.000200000000	-1.551698000000
C	3.564639000000	-0.000113000000	2.943199000000
H	2.210325000000	0.000289000000	4.622114000000
H	4.685968000000	-0.000660000000	1.109637000000
C	3.565753000000	0.000103000000	-2.942085000000
H	2.212078000000	-0.000303000000	-4.621516000000
H	4.686387000000	0.000653000000	-1.108097000000
H	4.456856000000	-0.000424000000	3.564396000000
H	4.458206000000	0.000414000000	-3.562942000000
Si	-0.056165000000	-0.000003000000	-0.000147000000
H	-4.221631000000	0.000014000000	0.001087000000

Cbz (S_0, Gas Phase) *E* = -517.470608899 Hartree			
N	0.000000000000	1.653832000000	0.000010000000
C	1.133686000000	0.855630000000	-0.000309000000
C	-1.133686000000	0.855630000000	0.000309000000
C	2.481722000000	1.221302000000	-0.000516000000
C	0.725231000000	-0.505236000000	0.000614000000
C	-2.481722000000	1.221302000000	0.000510000000
C	-0.725231000000	-0.505236000000	-0.000608000000
C	3.428756000000	0.199589000000	-0.000187000000
H	2.783634000000	2.265368000000	-0.000464000000
C	1.699364000000	-1.510871000000	0.000724000000
C	-3.428756000000	0.199589000000	0.000178000000
H	-2.783634000000	2.265368000000	0.000459000000
C	-1.699364000000	-1.510871000000	-0.000719000000
C	3.044918000000	-1.153136000000	0.000260000000
H	4.484856000000	0.455578000000	-0.000313000000
H	1.408600000000	-2.558241000000	0.000911000000
C	-3.044918000000	-1.153136000000	-0.000264000000
H	-4.484856000000	0.455578000000	0.000301000000
H	-1.408600000000	-2.558241000000	-0.000904000000
H	3.808563000000	-1.925687000000	0.000020000000
H	-3.808563000000	-1.925687000000	-0.000024000000
H	0.000000000000	2.661813000000	0.000004000000