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

Electronic Supplementary Information (ESI) for

The hypothiocyanite radical OSCN and isomers

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Table S1: Calculated harmonic IR frequencies (cm^{-1}) and intensities (km mol^{-1}, in parentheses) for various [N, C, O, S] isomers at the B3LYP/6-311+G(3df) level.

OSCN	OSNC	SOCN	ONCS	SCON
2227 (18)	2055 (337)	2327 (55)	2255 (113)	1242 (299)
1074 (30)	1145 (64)	1089 (72)	1330 (124)	1081 (206)
620 (49)	611 (101)	724 (41)	677 (3)	806 (13)
474 (1)	424 (7)	546 (2)	454 (1)	408 (3)
313 (3)	209 (< 1)	481 (9)	282 (<1)	246 (2)
186 (11)	134 (3)	202 (3)	227 (1)	125 (<1)

Table S2: Calculated harmonic IR frequencies (cm^{-1}) for SNCO and SONC at various levels.

SNCO			SONC		
B3LYP[a]	CCSD(T)[b]	CCSD(T)-F12[c]	B3LYP[a]	CCSD(T)[b]	CCSD(T)-F12[c]
2333 (1201)	2254	2276	2152 (147)	2098	2119
1447 (1)	1385	1402	886 (19)	880	899
670 (15)	699	706	735 (18)	749	761
547 (28)	590	591	451 (5)	441	449
492 (27)	508	510	256 (<1)	237	233
115 (11)	119	125	160 (<1)	148	151

[a] At the 6-311+G(3df) basis set. The calculated IR intensities (km mol^{-1}) are given in parentheses. [b] At the aug-cc-pV(T+d)Z basis set. [c] At the VTZ-F12 basis set.

Table S3: Calculated IR frequencies (cm^{-1}) of $CF_3S(O)CN$ isomers.

$CF_3S(O)CN$		CF_3OSCN	$CF_3S(O)NC$	CF_3SOCN
calculated[a]	observed[b]	calculated[a]	calculated[a]	calculated[a]
2283 (24)	2175.3	2245 (0.4)	2091 (424)	2344 (132)
1224 (263)	1236.9	1251 (344)	1238 (278)	1178 (250)
1206 (284)	1217.7	1193 (300)	1219 (186)	1172 (251)
1179 (<1)		1151 (604)	1191 (109)	1108 (249)
1094 (344)	1107.8	923 (43)	1106 (323)	1083 (203)
748 (11)	751.3	766 (24)	749 (6)	761 (14)
607 (51)	607.1	691 (14)	608 (100)	690 (30)
564 (12)		658 (1)	568 (31)	565 (2)
535 (10)		617 (4)	538 (13)	537 (3)
475 (13)		544 (14)	470 (27)	532 (5)
460 (12)		490 (3)	417 (15)	512 (8)
361 (4)		421 (1)	334 (<1)	458 (7)
296 (3)		399 (3)	286 (1)	325 (1)
272 (2)		371 (8)	235 (<1)	316 (1)
184 (8)		206 (3)	185 (4)	194 (4)
178 (8)		176 (5)	142 (4)	168 (1)
111 (3)		72 (2)	98 (1)	55 (2)
52 (4)		44 (2)	52 (<1)	47 (1)

[a]Calculated frequencies (unscaled) at the B3LYP/6-311++G(3df,3pd) level. [b]Observed band positions of the most intense site in solid Ar matrix.

Table S4: Results of the EDA-NOCV calculations of [O, S, C, N] isomers at BP86/TZ2P+ using the UCCSD(T)-F12/VTZ-F12 optimized geometries. Energy values in kcal/mol.

	OS-CN D/T	OS-NC D/T	SN-CO D/S	SO-CN D/T	SO-NC D/T
ΔE_{int}	-75.55	-61.26	-40.82	-62.76	-8.81
ΔE_{Pauli}	266.45	347.14	913.79	505.72	505.93
ΔE_{elstat}	-127.85	-151.72	-328.36	-208.46	-191.32
	37.4%	37.2%	34.4%	36.7%	37.2%
ΔE_{orb}	-214.15	-256.67	-626.25	-360.01	-323.41
	62.6%	62.8%	65.6%	63.3%	62.8%

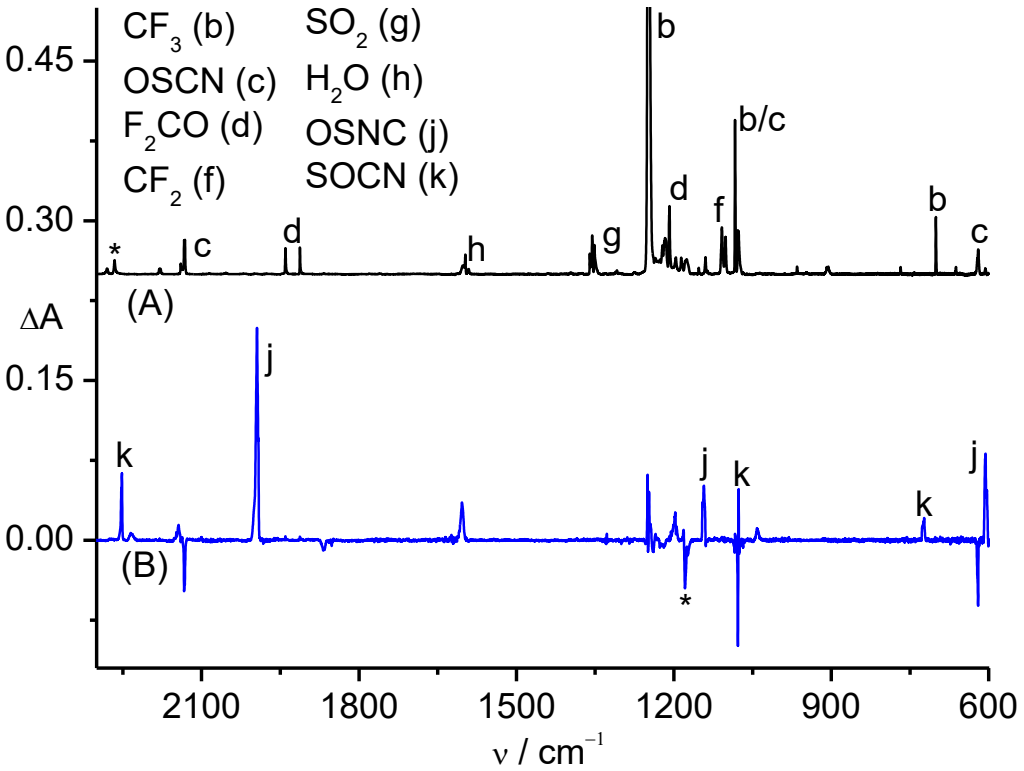

Figure S1: (A) IR spectrum of the flash vacuum pyrolysis (1000 K) products of $CF_3S(O)CN$ in solid N_2 matrix at 2.8 K. (B) IR difference spectrum showing the conversion from OSCN (c) to OSNC (j) and SOCN (k) upon UV light (365 nm) irradiation in solid N_2 matrix at 2.8 K. The IR bands for unknown species are marked with asterisks.

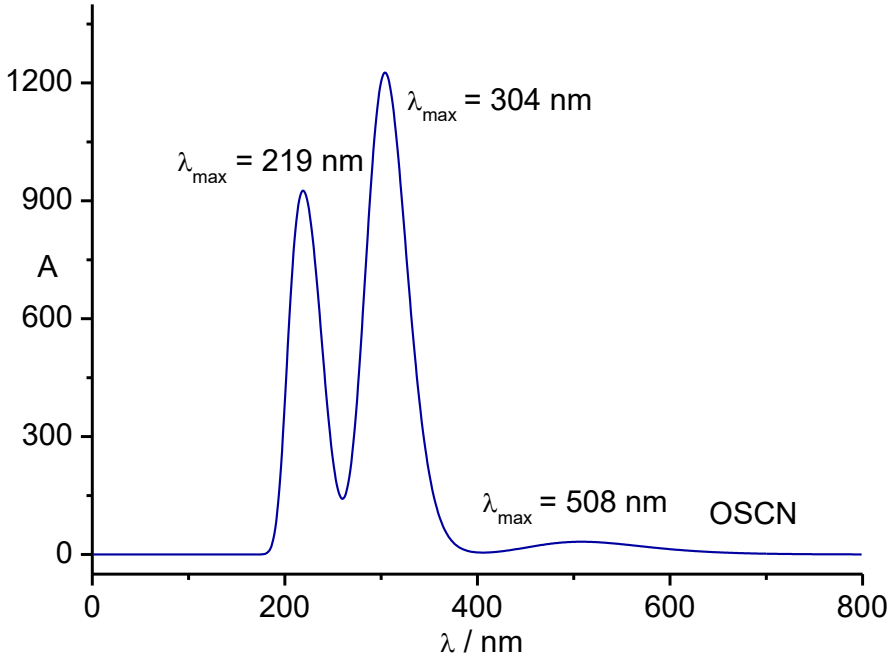

Figure S2: Calculated UV/Vis spectra of OSCN at the TD-B3LYP/6-311+G(3df) level.

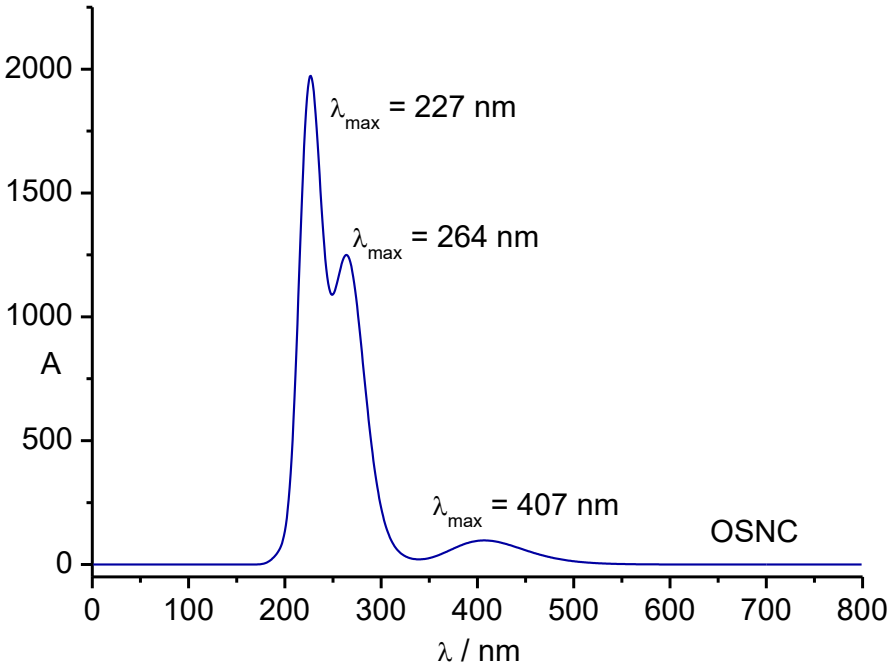

Figure S3: Calculated UV/Vis spectra of OSNC at the TD-B3LYP/6-311+G(3df) level.

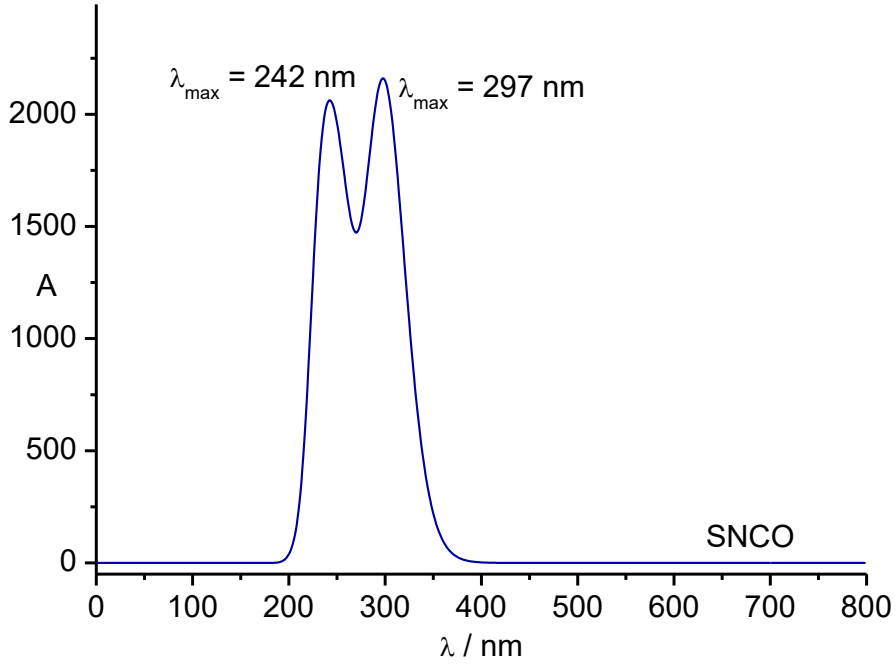

Figure S4: Calculated UV/Vis spectra of SNCO at the TD-B3LYP/6-311+G(3df) level.

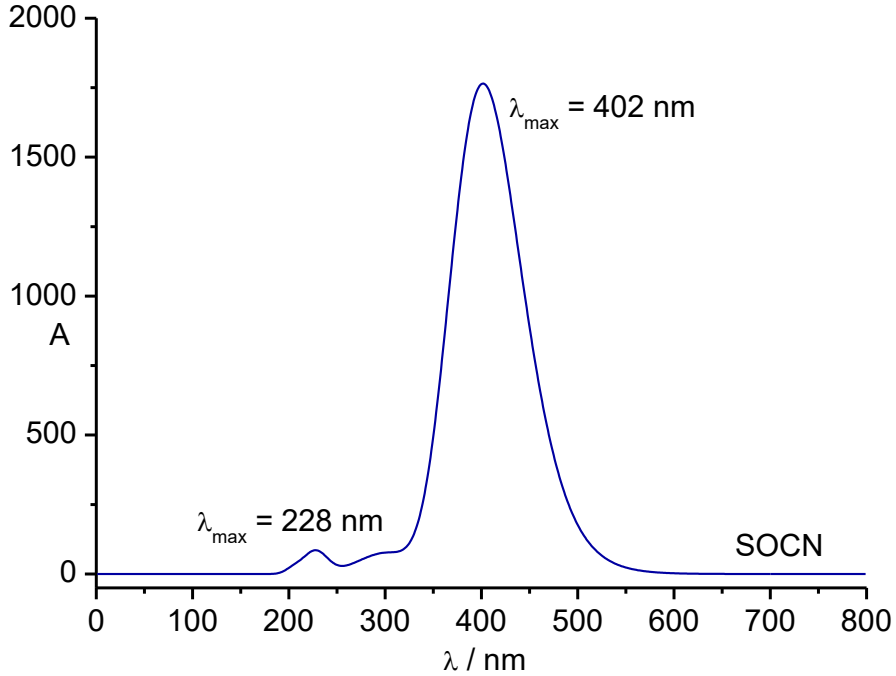

Figure S5: Calculated UV/Vis spectra of SOCN at the TD-B3LYP/6-311+G(3df) level.

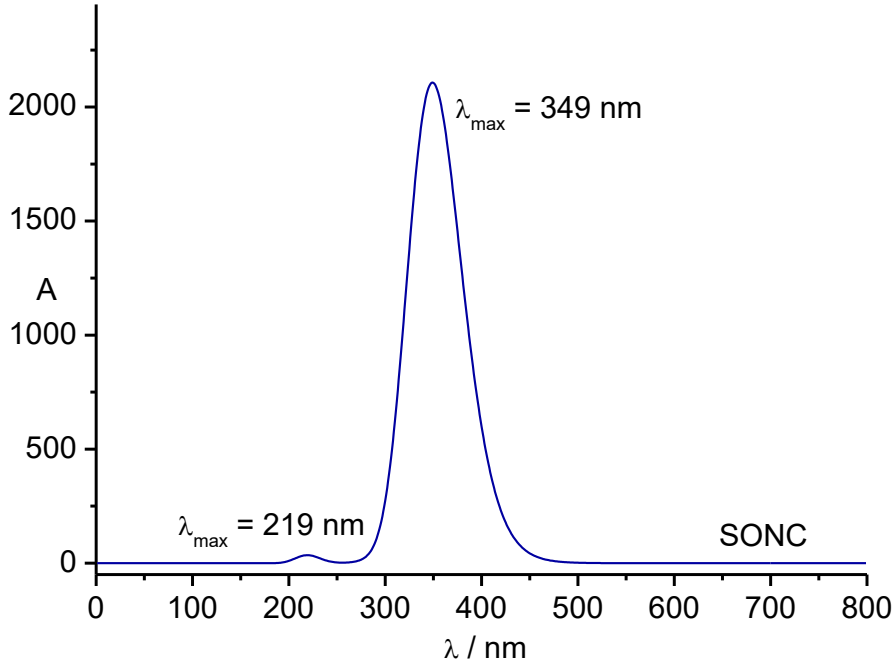

Figure S6: Calculated UV/Vis spectra of SONC at the TD-B3LYP/6-311+G(3df) level.

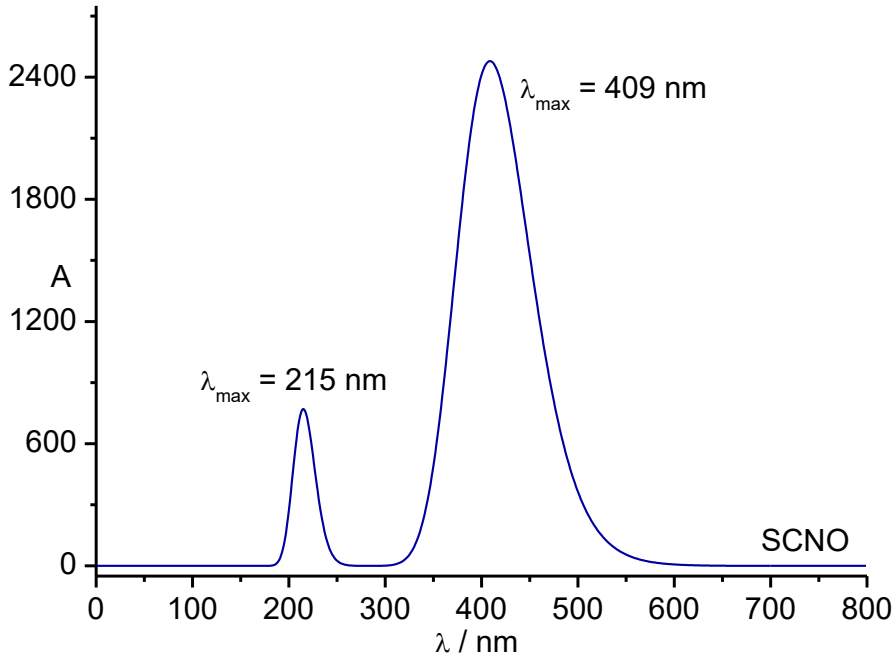

Figure S7: Calculated UV/Vis spectra of SCNO at the TD-B3LYP/6-311+G(3df) level

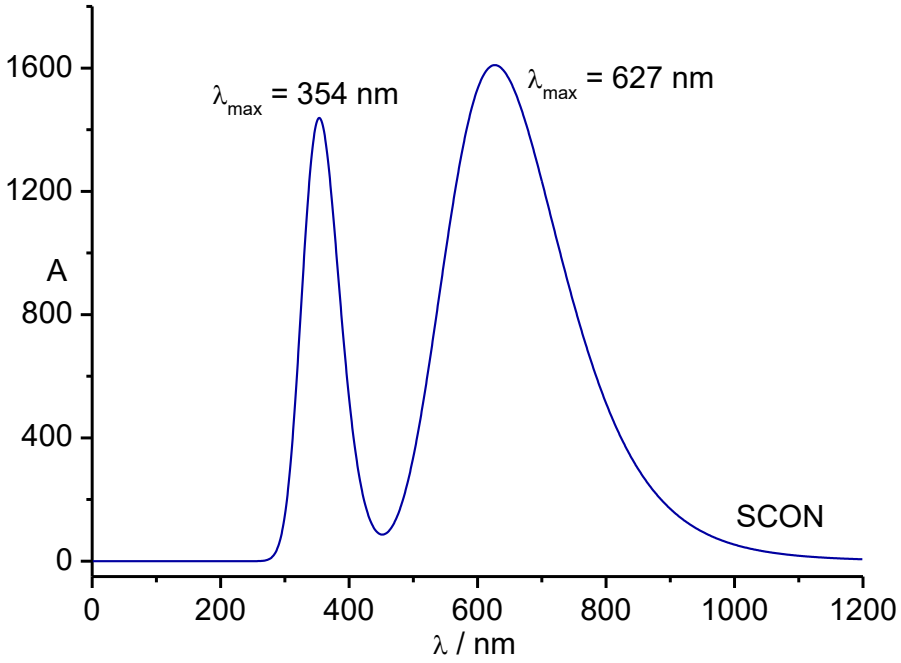

Figure S8: Calculated UV/Vis spectra of SCON at the TD-B3LYP/6-311+G(3df) level.

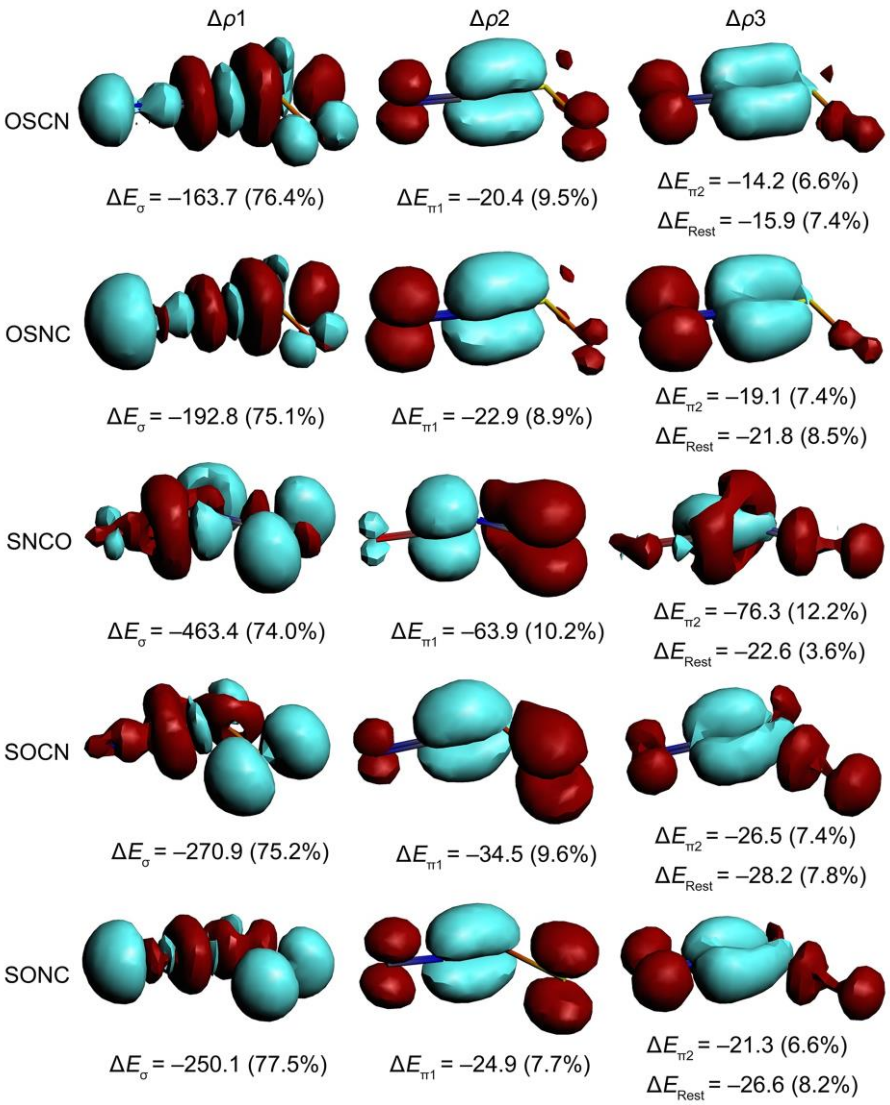

Figure S9: Plot of deformation densities $\Delta\rho$ of the pairwise orbital interactions between diatomic fragments in [S, O, C, N] isomers (see Table S3). The direction of the charge flow is red→blue

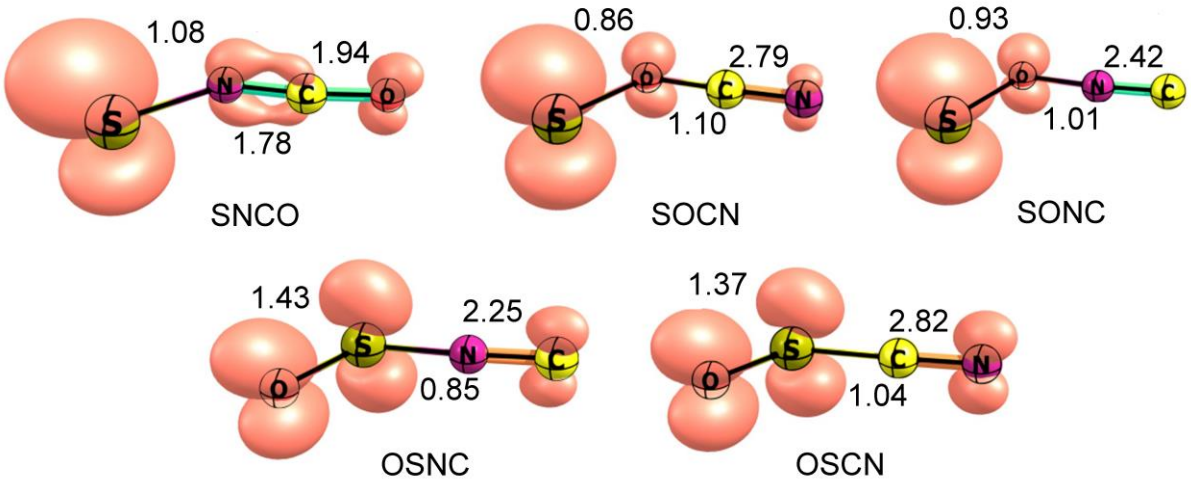

Figure S10: Calculated Wiberg bond indices of the [C, N, O, S] isomers at the UBP86/TZ2P+ level.

Calculated Atomic Coordinates (in Angstroms) and Energies (in Hartrees) for All Optimized Structures at the B3LYP/6-311+G(3df) Level of Theory.

OSCN

S	-0.61765400	-0.48556700	-0.00000700
O	-1.45013300	0.74777700	-0.00001300
C	1.04512400	0.00101800	0.00014800
N	2.17325500	0.25439300	-0.00009600

Zero-point correction=	0.011153
Thermal correction to Energy=	0.015392
Thermal correction to Enthalpy=	0.016336
Thermal correction to Gibbs Free Energy=	-0.016529
Sum of electronic and zero-point Energies=	-566.276588
Sum of electronic and thermal Energies=	-566.272350
Sum of electronic and thermal Enthalpies=	-566.271406
Sum of electronic and thermal Free Energies=	-566.304271

OSNC

S	0.56034700	-0.47385800	-0.00003700
O	1.43280600	0.70914600	0.00004000
N	-1.03769400	0.03796300	0.00000600
C	-2.19402300	0.27380400	0.00004000

Zero-point correction=	0.010436
Thermal correction to Energy=	0.014946
Thermal correction to Enthalpy=	0.015890
Thermal correction to Gibbs Free Energy=	-0.017568
Sum of electronic and zero-point Energies=	-566.253840
Sum of electronic and thermal Energies=	-566.249330
Sum of electronic and thermal Enthalpies=	-566.248385
Sum of electronic and thermal Free Energies=	-566.281844

SONC

S	-1.36281600	-0.25658400	0.00000000
O	0.00000000	0.70523600	0.00000000
C	2.26749200	-0.34277500	0.00000000
N	1.17144400	0.07430100	0.00000000

Zero-point correction=	0.010573
Thermal correction to Energy=	0.014930
Thermal correction to Enthalpy=	0.015874
Thermal correction to Gibbs Free Energy=	-0.017183
Sum of electronic and zero-point Energies=	-566.156944
Sum of electronic and thermal Energies=	-566.152587
Sum of electronic and thermal Enthalpies=	-566.151643
Sum of electronic and thermal Free Energies=	-566.184699

SNCO

N	0.00000000	0.32442700	0.00000000
O	2.30713600	-0.20509700	0.00000000
S	-1.58700600	-0.03287500	0.00000000
C	1.15583500	-0.01736700	0.00000000

Zero-point correction=	0.012770

Thermal correction to Energy=	0.016862
Thermal correction to Enthalpy=	0.017806
Thermal correction to Gibbs Free Energy=	-0.014310
Sum of electronic and zero-point Energies=	-566.303728
Sum of electronic and thermal Energies=	-566.299636
Sum of electronic and thermal Enthalpies=	-566.298691
Sum of electronic and thermal Free Energies=	-566.330808

SOCN

S	-1.39815500	-0.23822500	0.00000000
O	0.00000000	0.70115000	0.00000000
C	1.14998500	0.10710400	0.00000000
N	2.21008100	-0.34860300	0.00000000

Zero-point correction=	0.012239
Thermal correction to Energy=	0.016188
Thermal correction to Enthalpy=	0.017132
Thermal correction to Gibbs Free Energy=	-0.015141
Sum of electronic and zero-point Energies=	-566.242815
Sum of electronic and thermal Energies=	-566.238866
Sum of electronic and thermal Enthalpies=	-566.237922
Sum of electronic and thermal Free Energies=	-566.270195

SCNO

O	0.00000000	0.00000000	-2.34260100
N	0.00000000	0.00000000	-1.13221500
S	0.00000000	0.00000000	1.64846100
C	0.00000000	0.00000000	0.04848900

Zero-point correction=	0.012425
Thermal correction to Energy=	0.016660
Thermal correction to Enthalpy=	0.017604
Thermal correction to Gibbs Free Energy=	-0.012847
Sum of electronic and zero-point Energies=	-566.238998
Sum of electronic and thermal Energies=	-566.234764
Sum of electronic and thermal Enthalpies=	-566.233819
Sum of electronic and thermal Free Energies=	-566.264271

SCON

S	-1.54301200	0.10413000	0.00000000
C	0.00000000	0.41911300	0.00000000
O	1.05324200	-0.42035500	0.00000000
N	2.32317900	-0.11684600	0.00000000

Zero-point correction=	0.008903
Thermal correction to Energy=	0.013334
Thermal correction to Enthalpy=	0.014279
Thermal correction to Gibbs Free Energy=	-0.018699
Sum of electronic and zero-point Energies=	-566.134415
Sum of electronic and thermal Energies=	-566.129983
Sum of electronic and thermal Enthalpies=	-566.129039
Sum of electronic and thermal Free Energies=	-566.162017

TS1

S	-0.97687900	-0.22754800	0.00000100

O	0.19225800	1.12479200	-0.00000200
C	1.15557400	0.24113800	0.00000400
N	1.02265000	-0.97205700	-0.00000200

Zero-point correction=	0.010558
Thermal correction to Energy=	0.013943
Thermal correction to Enthalpy=	0.014888
Thermal correction to Gibbs Free Energy=	-0.016274
Sum of electronic and zero-point Energies=	-566.172205
Sum of electronic and thermal Energies=	-566.168820
Sum of electronic and thermal Enthalpies=	-566.167876
Sum of electronic and thermal Free Energies=	-566.199037

TS2

S	-0.93017000	-0.43561300	-0.00001200
O	-0.35824700	1.16664000	-0.00000400
C	0.72637000	-0.19402000	0.00008400
N	1.91292400	-0.17131300	-0.00004100

Zero-point correction=	0.009294
Thermal correction to Energy=	0.013044
Thermal correction to Enthalpy=	0.013988
Thermal correction to Gibbs Free Energy=	-0.017916
Sum of electronic and zero-point Energies=	-566.187514
Sum of electronic and thermal Energies=	-566.183763
Sum of electronic and thermal Enthalpies=	-566.182819
Sum of electronic and thermal Free Energies=	-566.214723

TS3

S	0.44023400	-0.47665900	-0.03471700
O	1.38886900	0.63127700	0.01912600
C	-1.31225500	0.13561300	0.66369100
N	-1.46873800	0.25180700	-0.51138400

Zero-point correction=	0.009374
Thermal correction to Energy=	0.013439
Thermal correction to Enthalpy=	0.014383
Thermal correction to Gibbs Free Energy=	-0.018060
Sum of electronic and zero-point Energies=	-566.223585
Sum of electronic and thermal Energies=	-566.219519
Sum of electronic and thermal Enthalpies=	-566.218575
Sum of electronic and thermal Free Energies=	-566.251018

TS4

S	-0.99357000	-0.37904300	-0.00037800
O	-0.11844700	1.12971200	-0.00052700
N	0.74897700	-0.09569300	0.00317700
C	1.93364300	-0.38386100	-0.00199700

Zero-point correction=	0.008260
Thermal correction to Energy=	0.012174
Thermal correction to Enthalpy=	0.013118
Thermal correction to Gibbs Free Energy=	-0.019017
Sum of electronic and zero-point Energies=	-566.094316
Sum of electronic and thermal Energies=	-566.090402

Sum of electronic and thermal Enthalpies= -566.089458
Sum of electronic and thermal Free Energies= -566.121593

SN

N	0.00000000	0.00000000	-1.03673800
S	0.00000000	0.00000000	0.45357300

Zero-point correction= 0.002872
Thermal correction to Energy= 0.005245
Thermal correction to Enthalpy= 0.006189
Thermal correction to Gibbs Free Energy= -0.018467
Sum of electronic and zero-point Energies= -452.915919
Sum of electronic and thermal Energies= -452.913546
Sum of electronic and thermal Enthalpies= -452.912602
Sum of electronic and thermal Free Energies= -452.937258

singlet SO

S	0.00000000	0.00000000	0.49625300
O	0.00000000	0.00000000	-0.99250600

Zero-point correction= 0.002635
Thermal correction to Energy= 0.005016
Thermal correction to Enthalpy= 0.005960
Thermal correction to Gibbs Free Energy= -0.018194
Sum of electronic and zero-point Energies= -473.378933
Sum of electronic and thermal Energies= -473.376552
Sum of electronic and thermal Enthalpies= -473.375608
Sum of electronic and thermal Free Energies= -473.399761

triplet SO

S	0.00000000	0.00000000	0.49611100
O	0.00000000	0.00000000	-0.99222100

Zero-point correction= 0.002636
Thermal correction to Energy= 0.005017
Thermal correction to Enthalpy= 0.005961
Thermal correction to Gibbs Free Energy= -0.019229
Sum of electronic and zero-point Energies= -473.424353
Sum of electronic and thermal Energies= -473.421973
Sum of electronic and thermal Enthalpies= -473.421029
Sum of electronic and thermal Free Energies= -473.446219

CN

C	0.00000000	0.00000000	-0.62576400
N	0.00000000	0.00000000	0.53636900

Zero-point correction= 0.004901 (Hartree/Particle)
Thermal correction to Energy= 0.007262
Thermal correction to Enthalpy= 0.008206
Thermal correction to Gibbs Free Energy= -0.014771
Sum of electronic and zero-point Energies= -92.739756
Sum of electronic and thermal Energies= -92.737396
Sum of electronic and thermal Enthalpies= -92.736451
Sum of electronic and thermal Free Energies= -92.759429

CO

O	0.00000000	0.00000000	0.48191000
C	0.00000000	0.00000000	-0.64254600

Zero-point correction=	0.005050
Thermal correction to Energy=	0.007411
Thermal correction to Enthalpy=	0.008355
Thermal correction to Gibbs Free Energy=	-0.014066
Sum of electronic and zero-point Energies=	-113.351743
Sum of electronic and thermal Energies=	-113.349382
Sum of electronic and thermal Enthalpies=	-113.348438
Sum of electronic and thermal Free Energies=	-113.370858

$CF_3S(O)NC$

C	0.96949800	-0.24427100	0.02588800
F	1.98788700	0.56234600	-0.26336800
F	0.97479400	-0.51701500	1.31724500
F	1.08008300	-1.36453000	-0.68024700
S	-0.61368100	0.69458600	-0.50172600
O	-0.75290000	1.79951800	0.42840100
N	-1.61002900	-0.59839800	-0.00101800
C	-2.51492700	-1.33038500	0.18158700

Zero-point correction=	0.026264
Thermal correction to Energy=	0.034471
Thermal correction to Enthalpy=	0.035415
Thermal correction to Gibbs Free Energy=	-0.007700
Sum of electronic and zero-point Energies=	-903.991308
Sum of electronic and thermal Energies=	-903.983101
Sum of electronic and thermal Enthalpies=	-903.982157
Sum of electronic and thermal Free Energies=	-904.025272

CF_3OSCN

C	-1.22088200	0.15958800	0.01069500
F	-1.73715000	-0.72364900	-0.84688100
F	-2.16642400	0.55801700	0.84506000
F	-0.78017600	1.20324400	-0.68889700
S	1.10531600	-1.03895400	-0.01234900
O	-0.22728400	-0.40188800	0.78626300
C	2.16026700	0.27928100	0.01069800
N	2.95009500	1.12380500	-0.00063100

Zero-point correction=	0.027835
Thermal correction to Energy=	0.035408
Thermal correction to Enthalpy=	0.036352
Thermal correction to Gibbs Free Energy=	-0.005896
Sum of electronic and zero-point Energies=	-904.049559
Sum of electronic and thermal Energies=	-904.041987
Sum of electronic and thermal Enthalpies=	-904.041043
Sum of electronic and thermal Free Energies=	-904.083291

Calculated Atomic Coordinates (in Angstroms) and Energies (in Hartrees) for All Optimized Structures at the CCSD(T)/aug-cc-PV(T+D)Z and CCSD(T)-F12/VTZ-F12 Level of Theory.

OSCN

UCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-565.51030924

S	0.0803608034	-0.3640140924	-0.0339056301
C	-0.2393613493	0.4591940665	1.4706226965
O	1.4067287167	0.1024690373	-0.5189150705
N	-0.5123351708	0.9781049886	2.4822020040

UCCSD(T)-F12/VTZ-F12 ENERGY=-565.58571616

S	0.0825416712	-0.3600143146	-0.0299701518
C	-0.2363954861	0.4592262158	1.4682038010
O	1.4003070932	0.1018312015	-0.5141681229
N	-0.5110602783	0.9747108973	2.4759384737

OSNC

UCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-565.48591456

C	1.6082377006	1.2467571408	1.9699790098
N	1.0615422971	0.4054092893	1.3292174049
S	0.2020743224	-0.7998589714	0.5210400927
O	0.8457996799	-1.0235494587	-0.7841565074

UCCSD(T)-F12/VTZ-F12 ENERGY=-565.56146293

C	1.6035151509	1.2406465851	1.9664052331
N	1.0623025294	0.4029683389	1.3239866164
S	0.2075839322	-0.7948558275	0.5216011099
O	0.8442523876	-1.0200010965	-0.7759129593

SNCO

UCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-565.52908563

C	0.6807537658	-0.5029105953	0.3372813835
N	0.7639011959	0.1668429383	1.3608854913
S	1.7609049230	1.3597757796	1.9367688321
O	0.4572651154	-1.2181401227	-0.5595637070

UCCSD(T)-F12/VTZ-F12 ENERGY=-565.60279507

C	0.6818361946	-0.5026039961	0.3364334953
N	0.7749770762	0.1706009454	1.3508273536
S	1.7530879828	1.3556072702	1.9411808564
O	0.4529237464	-1.2180362195	-0.5530697053

SOCN

UCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-565.47773970

C	0.5047841807	-0.0004490710	0.3605474304
O	-0.1038023773	-0.1427781176	1.5143463168
N	1.0578505189	0.0545695436	-0.6641262066
S	-0.7234403223	1.2644116450	2.1892364595

UCCSD(T)-F12/VTZ-F12 ENERGY=-565.54989735

C	0.5038326287	0.0000051118	0.3621302860
O	-0.1033796630	-0.1383886921	1.5121641609
N	1.0546207827	0.0552339965	-0.6584588359
S	-0.7196817485	1.2589035839	2.1841683890

SONC

UCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-565.38964742

N	0.0000000000	0.0520092322	1.1739533353
C	0.0000000000	-0.4091781105	2.2650866045
O	0.0000000000	0.7308159925	0.0102666862
S	0.0000000000	-0.2346597149	-1.3451596759

UCCSD(T)-F12/VTZ-F12 ENERGY=-565.46092431

N	0.0000000000	0.0542320055	1.1716354899
C	0.0000000000	-0.4086705496	2.2567032214
O	0.0000000000	0.7267430291	0.0112646075
S	0.0000000000	-0.2333170857	-1.3354563686

TS1

RCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-565.40752578

S	0.0093750633	0.0000025424	-0.0342634146
O	-0.0216006473	-0.0000042404	1.7512225359
C	1.2945232270	0.0000016878	1.7264794381
N	2.0238893571	0.0000110103	0.7379024406

RCCSD(T)-F12/VTZ-F12 ENERGY=-565.48048286

S	0.0106564757	0.0000104011	-0.0264748009
O	-0.0185679670	-0.0000167730	1.7442101171
C	1.2931879108	0.0000029425	1.7232664479
N	2.0209105805	0.0000144295	0.7403392359

TS3

RCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-565.45533146

C	-0.6726345190	0.1353483061	-1.2974544283
N	0.5134648599	0.2535452372	-1.4759557714
S	0.0361755505	-0.4795525194	0.4400672547
O	-0.0170458389	0.6373647259	1.3843293284

RCCSD(T)-F12/VTZ-F12 ENERGY=-565.53070365

C	-0.6709132822	0.1335311183	-1.2748961251
N	0.5071094377	0.2538302324	-1.4719833936
S	0.0374863695	-0.4755676015	0.4336057054
O	-0.0154007859	0.6304943389	1.3768646475

TS4

CCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-565.32390277

S	-0.0046317282	-0.0008866704	-0.0110217689
O	-0.0116654601	-0.0006930289	1.7471320756
N	1.3666037148	0.0033172271	1.1343006740
C	2.5493714735	0.0065334722	1.4577050193

CCSD(T)-F12/VTZ-F12 ENERGY=-565.39567581

S	-0.0001146013	-0.0008384504	-0.0036990289
O	-0.0033151277	-0.0006431086	1.7411853328
N	1.3617496851	0.0031697732	1.1336017380
C	2.5413580439	0.0065827857	1.4570279581

CN

UCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-92.57279337

C	0.0721684324	0.0054673055	0.0000000000
N	1.2478315676	0.0945326945	0.0000000000

UCCSD(T)-F12/VTZ-F12 ENERGY=-92.60041792

C	0.0748596929	0.0056711889	0.0000000000
N	1.2451403071	0.0943288111	0.0000000000

singlet SO

RCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-472.79013550

S	-0.0901745700	-0.0068314068	0.0000000000
O	1.4101745700	0.1068314068	0.0000000000

RCCSD(T)-F12/VTZ-F12 ENERGY=-472.83465433

S	-0.0847484411	-0.0064203364	0.0000000000
O	1.4047484411	0.1064203364	0.0000000000

triplet SO

RCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-472.82625571

S	-0.0841755346	-0.0063769344	0.0000000000
O	1.4041755346	0.1063769344	0.0000000000

RCCSD(T)-F12/VTZ-F12 ENERGY=-472.87012350

S	-0.0791709341	-0.0059977980	0.0000000000
O	1.3991709341	0.1059977980	0.0000000000

CO

RCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-113.16219363

C	0.0936102726	0.0070916873	0.0000000000
O	1.2263897274	0.0929083127	0.0000000000

RCCSD(T)-F12/VTZ-F12 ENERGY=-113.19975369

C	0.0962882363	0.0072945634	0.0000000000
O	1.2237117637	0.0927054366	0.0000000000

SN

UCCSD(T)/AUG-CC-PV(T+D)Z ENERGY=-452.34279935

S	-0.0904340993	-0.0068510681	0.0000000000
N	1.4104340993	0.1068510681	0.0000000000

UCCSD(T)-F12/VTZ-F12 ENERGY=-452.37822468

S	-0.0858582940	-0.0065044162	0.0000000000
N	1.4058582940	0.1065044162	0.0000000000