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

Supporting Information: MS-CASPT2 Studies on Mechanistic Photophysics of Tellurium-Substituted Guanine and Cytosine

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1. Active Spaces for TeC and TeG Systems

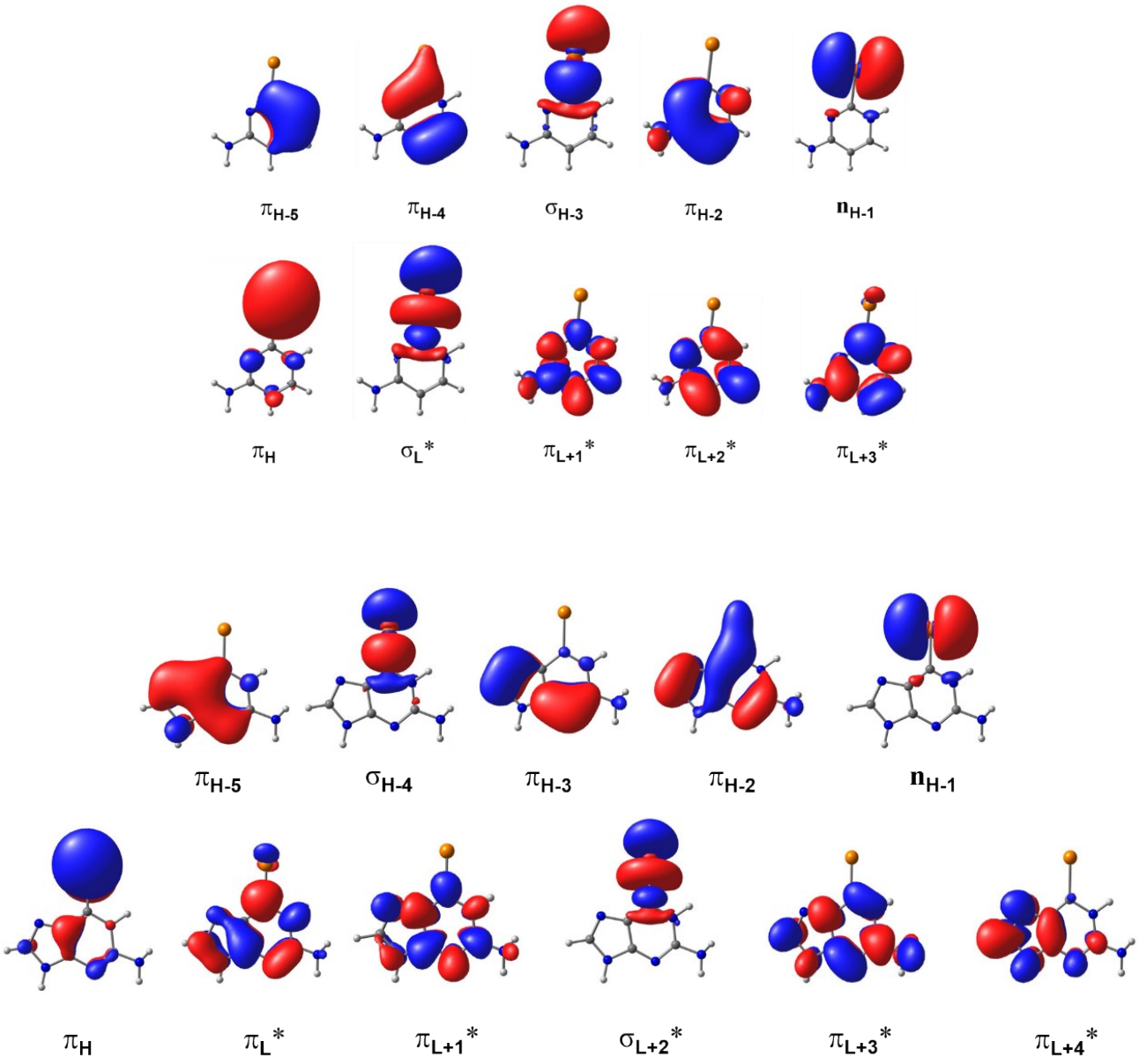


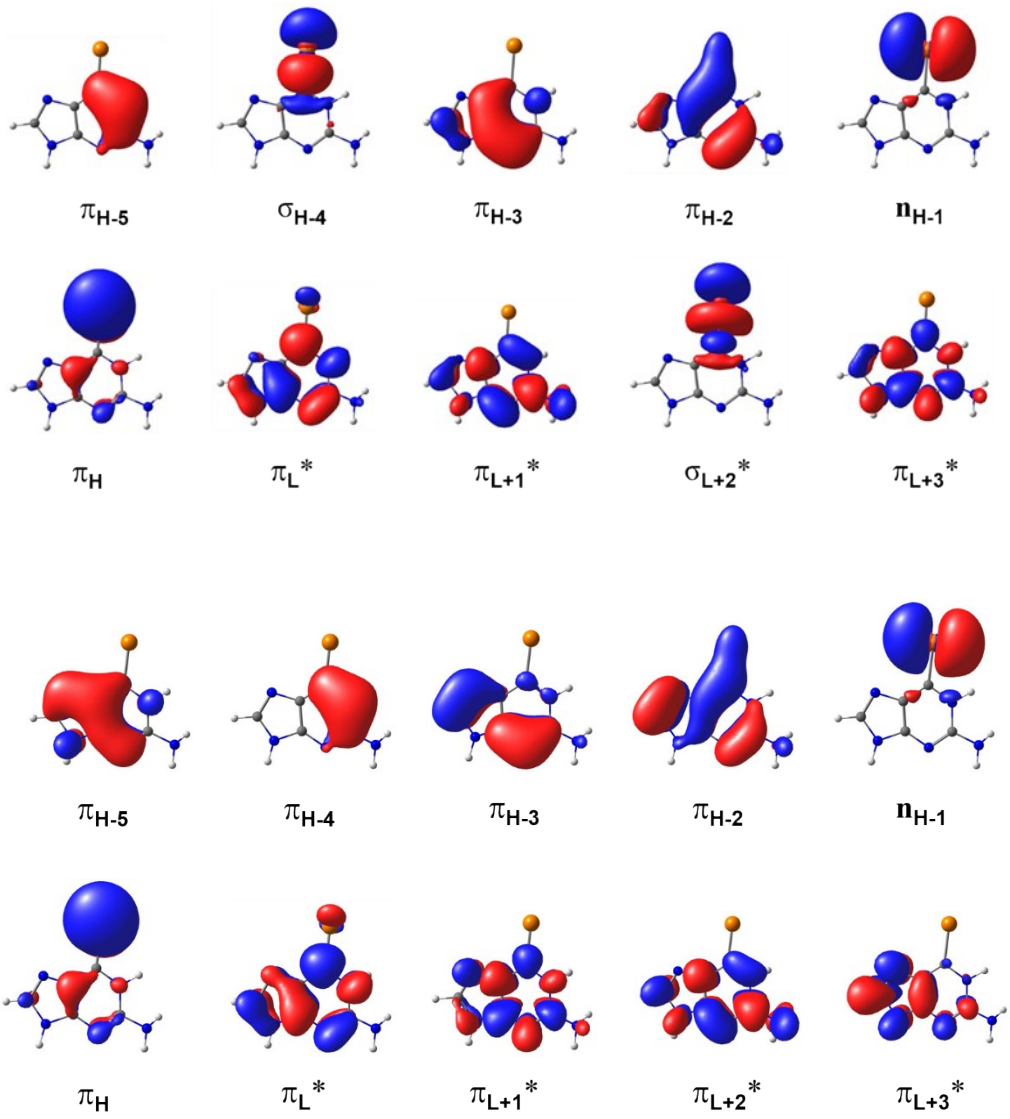
Figure S1. Molecular orbitals of TeC (top) and TeG (bottom) used as active spaces in the MS-CASPT2 calculations.

2. The Choice of Active Spaces for TeG

Table S1. Vertical excitation energies at MS-CASPT2-optimized S_0 minima of TeG with different active spaces.

States	$(12,10)^{top}$	$(12,10)^{middle}$	$(14,12)^{bottom}$
$S_1(n\pi^*)$	53.9	58.4	52.8
$S_2(\pi\pi^*)$	65.9	67.0	64.3
$T_1(\pi\pi^*)$	49.1	52.7	47.4
$T_2(n\pi^*)$	53.3	57.5	52.2
$T_3(\pi\pi^*)$	79.5	84.1	78.9

The superscripts of "top", "middle" and "bottom" refer to the different active spaces of TeG in Fig. S2.



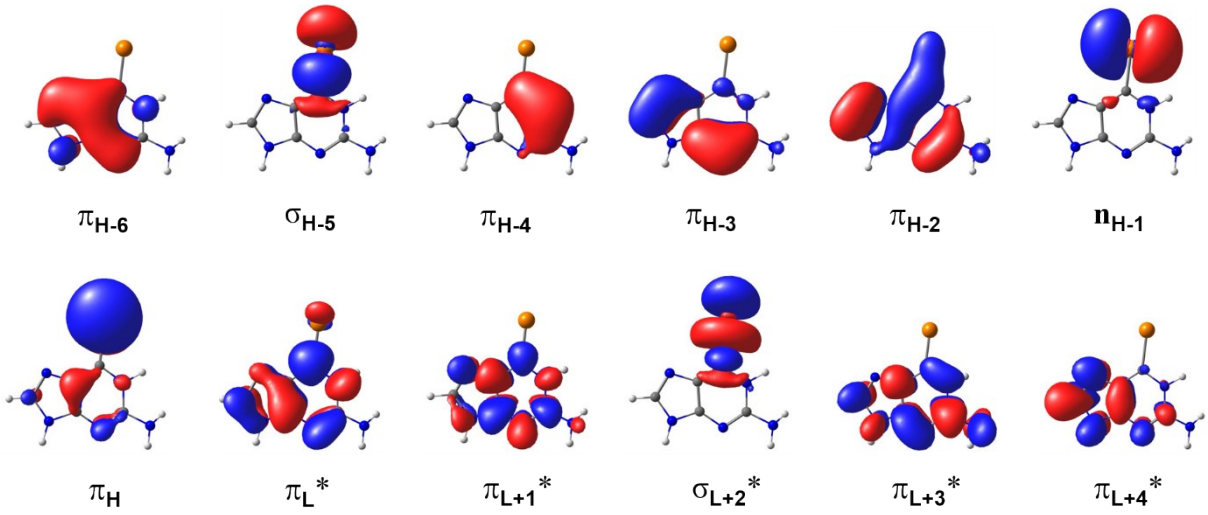


Figure S2. Molecular orbitals of TeG used as different active spaces (12,10)-(top), (12,10)-(middle), (14,12)-(bottom) in the MS-CASPT2 calculations.

3. The Explicit Spin-Orbit Coupled Calculations

Table S2. The absorption energies and oscillator strengths of $S_0 \rightarrow T_n$ calculated with different density functionals.

Structures	States	cam-b3lyp		wb97x-v	
		Energy (eV)	Osc.	Energy (eV)	Osc.
TeG	S_1	2.47	$0.17*10^{-04}$	2.65	$0.14*10^{-04}$
	S_2	3.29	0.32	3.36	0.34
	T_1	1.65	$0.30*10^{-05}$	1.69	$0.35*10^{-05}$
	T_2	2.16	$0.89*10^{-02}$	2.35	$0.12*10^{-01}$
	T_3	3.38	$0.16*10^{-02}$	3.62	$0.12*10^{-03}$
TeC	S_1	2.71	$0.67*10^{-04}$	2.93	$0.66*10^{-04}$
	S_2	2.95	$0.22*10^{-01}$	3.42	0.13
	T_1	2.00	$0.13*10^{-04}$	2.12	$0.14*10^{-04}$
	T_2	2.40	$0.68*10^{-02}$	2.64	$0.72*10^{-02}$
	T_3	2.67	$0.25*10^{-03}$	3.07	$0.76*10^{-03}$

Oscillator strengths are evaluated by the TD-DFT method with the zero-order regular approximation to account for the scalar relativistic effects.

4. Comparison with Different Chalcogen Substitutions

Table S3.Vertical excitation energies at S_0 minima of guanine and cytosine with different chalcogen atom substitutions (units: eV).

States	TeG[a]	SeG[b]	TG[c]	G[d]	TeC[a]	TC[e]	C[f]
$S_1(n\pi^*)$	2.32	2.61	3.36	**4.93**($\pi\pi^*$)	2.52	3.65	**4.68**($\pi\pi^*$)
$S_2(\pi\pi^*)$	**2.84**	**3.39**	**4.05**	5.54($n\pi^*$)	**2.78**	**3.74**	5.12($n\pi^*$)
$T_1(\pi\pi^*)$	2.14	2.40	3.10	-	2.35	3.37	-
$T_2(n\pi^*)$	2.30	2.56	3.31	-	2.48	3.47($\pi\pi$*)	-
$T_3(\pi\pi^*)$	3.51	-	4.24	-	2.72	3.64($n\pi$*)	-

[a] This work. [b] *ACS Omega* 2019, 4, 9769−9777. [c] *Chem. Commun.*2012, 48, 2134–2136. [d] *J. Am. Chem. Soc.* 2008, 130, 2473-2484. [e] *Nat. Commun.* 2016, 7, 13077. [f]*J. Chem. Phys.* 2008, 128, 134110.

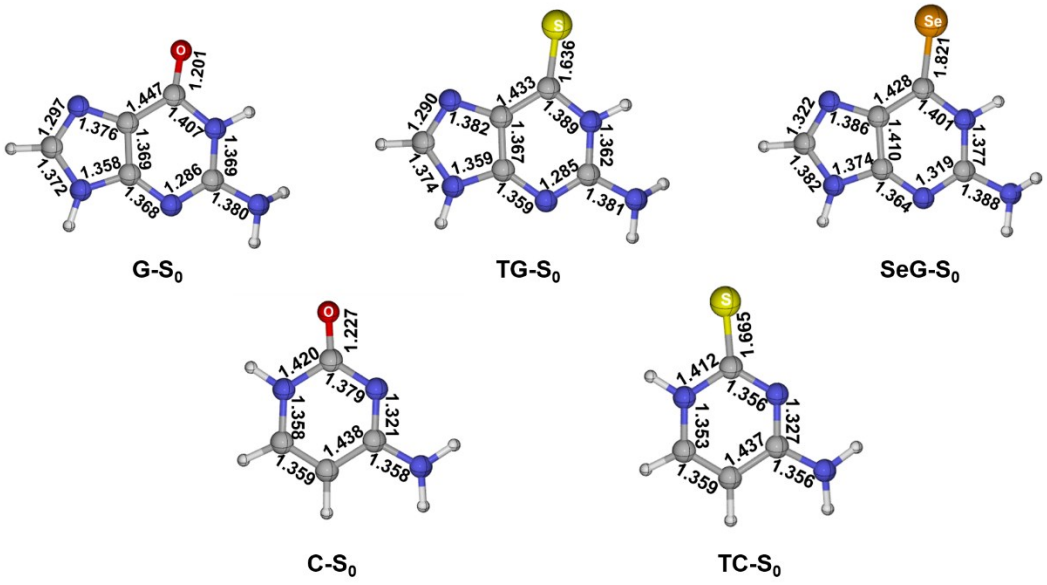


Figure S3. Ground-state equilibrium structures of G (top) and C (bottom) with different heavy atom substitutions. Also shown are the selected bond lengths (in Å).

Table S4. The spin-orbit constants (cm^{-1}) and intersystem crossing rates (s^{-1}) of guanine and cytosine with different chalcogen atom substitutions in the Franck-Condon approximation based on the MS-CASPT2 calculations.

Systems	Structures	States	SOC	ISC
TC[a]	MECP $^1n\pi^*/^3\pi\pi^*$	$^1n\pi^*/^3\pi\pi^*$	160	$3.75*10^{14}$
	MECP $^1\pi\pi^*/^3n\pi^*$	$^1\pi\pi^*/^3n\pi^*$	170	$4.24*10^{14}$
TeC[b]	$(S_2/S_1/T_2/T_1)_P$	S_2/T_2	992	$1.70*10^{16}$
	$(S_2/S_1/T_2)_T$	S_2/T_2	849	$5.80*10^{14}$
	$(T_2/T_1/S_0)_T$	T_1/S_0	1028	$3.60*10^{15}$
	T_{3P}	S_2/T_3	292	$1.50*10^{14}$
	S_{1P}	S_1/T_1	768	$4.00*10^{15}$
		S_1/T_2	619	$3.20*10^{15}$
	S_{1T}	S_1/T_1	795	$7.90*10^{14}$
		S_1/T_2	591	$7.40*10^{14}$
TG[c]	S_0	S_2/T_2	100	$2.10*10^{12}$
	S_1/T_2	S_1/T_2	200	$2.93*10^{13}$
	T_1/S_0	$T_1(^3n\pi^*)/S_0$	270	$2.14*10^{13}$
	T_1/S_0	$T_1(^3\pi\pi^*)/S_0$	12	$2.64*10^{11}$
SeG in gas phase[d]	S_1-MIN	S_1/T_1	437	$4.67*10^{14}$
		S_1/T_2	14	$1.44*10^{12}$
	$S_2/S_1/T_2$	S_2/T_2	435	$1.39*10^{15}$
	S_0/T_1	T_1/S_0	252	$7.16*10^{13}$
SeG in water [e]	$S_2/S_1/T_2$	S_2/T_2	440	$5.68*10^{14}$
	$S_1/T_1/T_2$	S_1/T_1	380	$3.03*10^{14}$
		S_1/T_2	155	$5.87*10^{13}$
	T_1/S_0	T_1/S_0	283	$3.56*10^{13}$
SeG in DNA [e]	S_1-MIN	S_1/T_1	399	$1.17*10^{14}$
		S_1/T_2	93	$6.34*10^{12}$
	T_1/S_0	T_1/S_0	273	$2.73*10^{14}$
TeG[b]	$(S_2/S_1/T_2)_P$	S_2/T_2	906	$2.10*10^{15}$
	$(T_1/S_0)_T$	T_1/S_0	694	$2.50*10^{14}$
	S_{1P}	S_1/T_1	888	$1.20*10^{15}$
		S_1/T_2	359	$1.10*10^{15}$
	S_{1T}	S_1/T_1	953	$1.20*10^{15}$
		S_1/T_2	20	$1.00*10^{12}$

[a] *Nat. Commun.* 2016, 7, 13077. [b] This work. [c] *Chem. Commun.*2012, 48, 2134–2136. *Chem. Sci.* 2014, 5, 1336–1347. [d] *ACS Omega* 2019, 4, 9769−9777. [e] *J. Phys. Chem. B* 2021,125,1778−1789

5. Additional Proposed Excited-State Relaxation Paths of TeG and TeC Calculated at the MS-CASPT2 Level

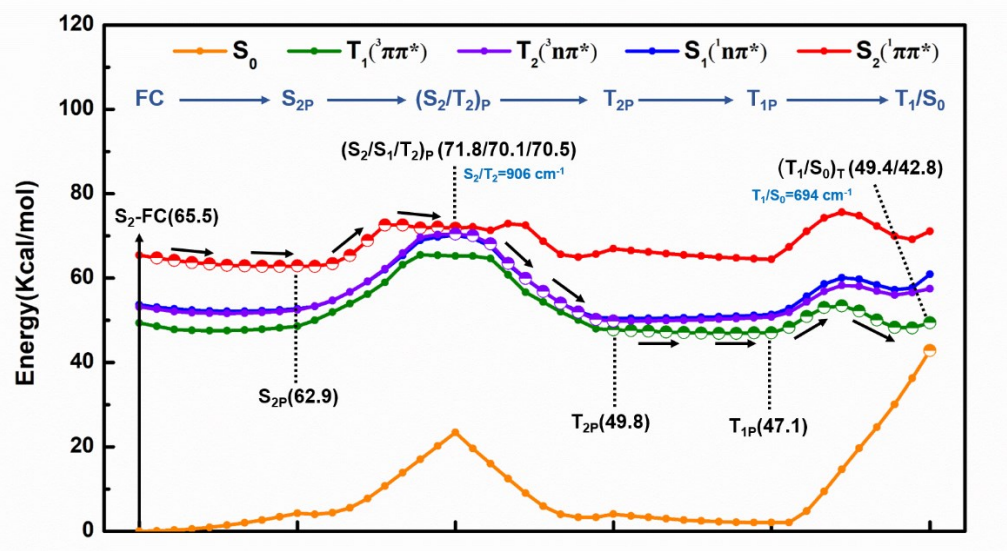


Figure S4. The proposed excited-state relaxation pathways of TeG based on the MS-CASPT2 calculated LIIC paths (in kcal/mol).

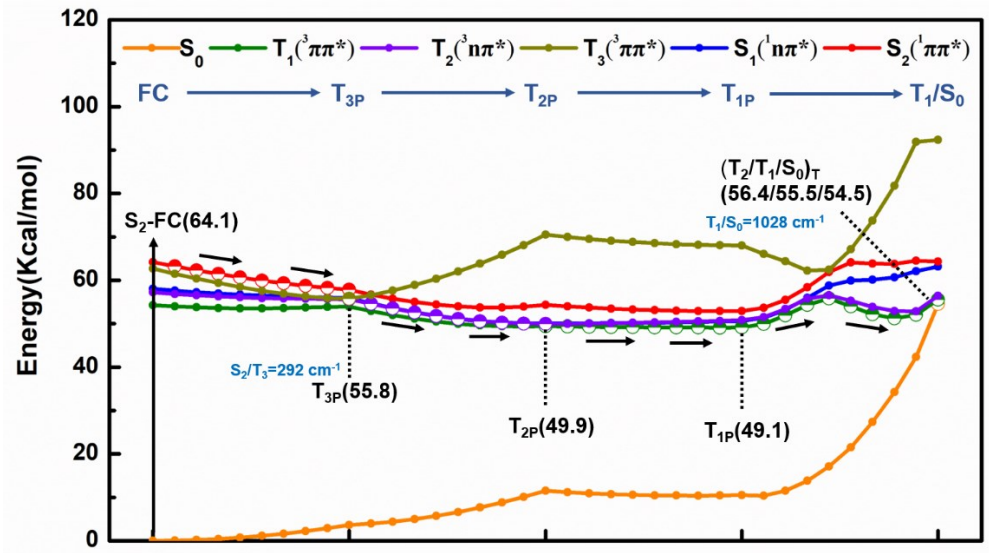


Figure S5. The proposed excited-state relaxation pathways of TeC based on the MS-CASPT2 calculated LIIC paths (in kcal/mol).

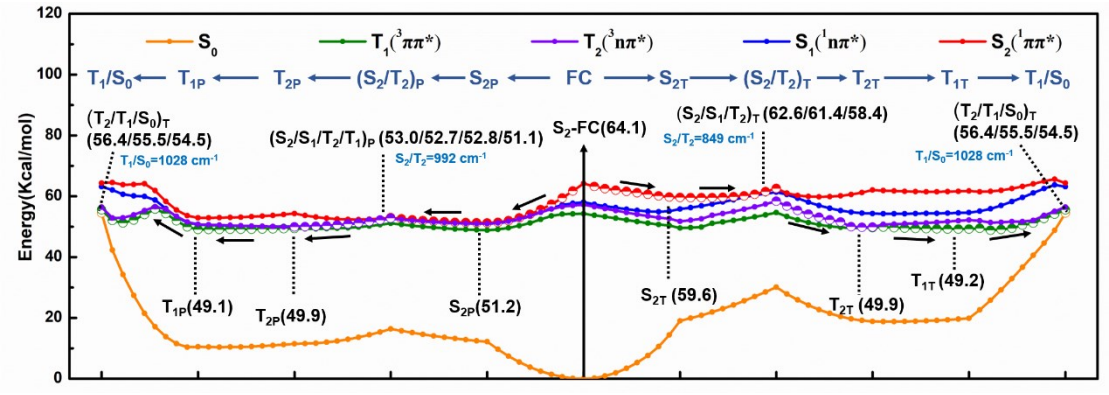


Figure S6. The proposed excited-state relaxation pathways of TeC based on the MS-CASPT2 calculated LIIC paths (in kcal/mol).

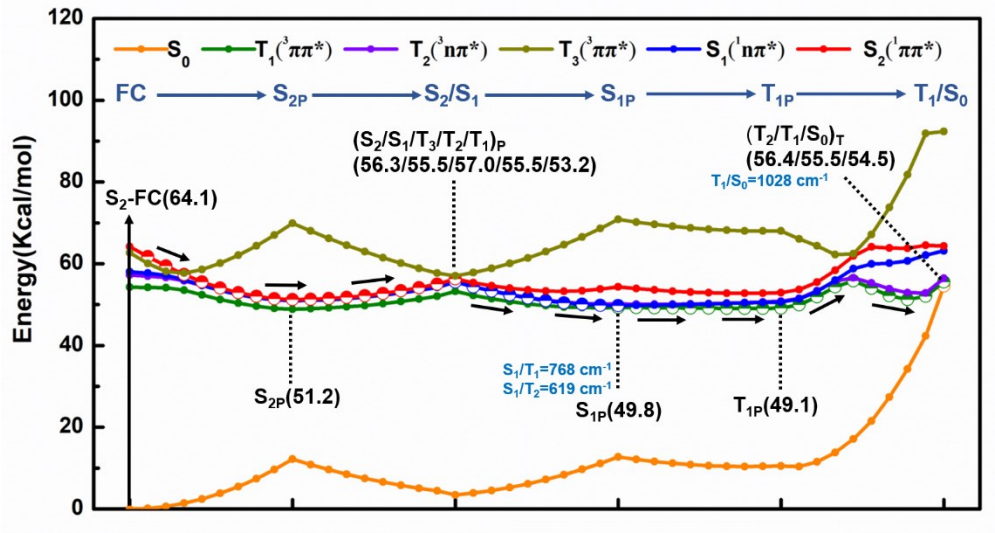


Figure S7. The proposed excited-state relaxation pathways of TeC based on the MS-CASPT2 calculated LIIC paths (in kcal/mol).

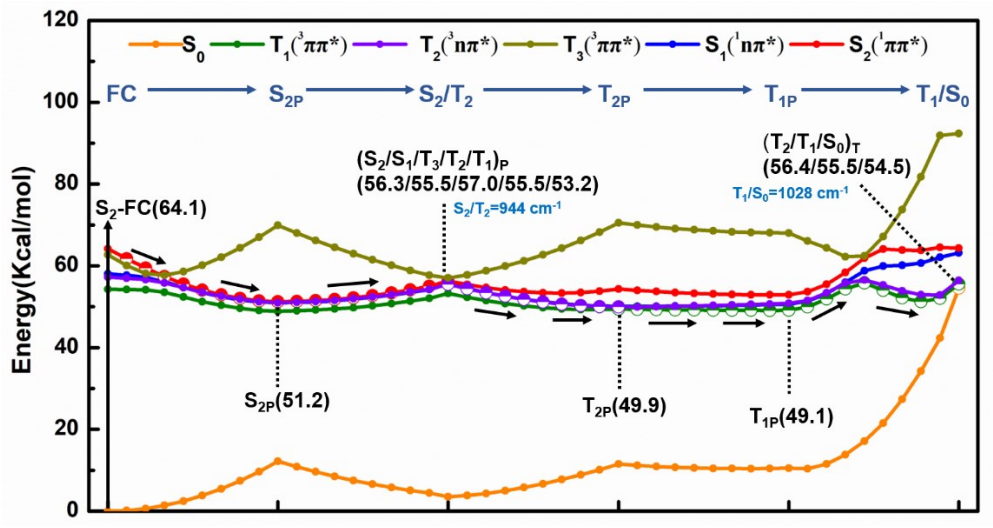


Figure S8. The proposed excited-state relaxation pathways of TeC based on the MS-CASPT2 calculated LIIC paths (in kcal/mol).

6. Cartesian Coordinates for Critical Structures Optimized at the MS-CASPT2 Level (Unit: Angstrom)

TeG

S_0

C	-2.35911727	-0.55592892	0.02671339
C	-0.95418872	-0.41040103	-0.01460104
C	-0.99696900	1.80318030	0.04049956
C	-3.15118232	0.60416823	0.12098135
C	-1.56904516	-2.52861933	-0.09028575
H	-2.88692519	2.62267474	0.23103670
H	0.50494729	-1.95177130	-0.12905934
N	-2.36665327	1.75853835	0.10714457
N	-0.42031171	3.05969860	0.14684376
H	0.56994432	3.01445893	-0.06405144
H	-0.87658700	3.77735693	-0.40519712
N	-0.22785140	0.72371813	-0.01233671
N	-2.71676425	-1.89401487	-0.02019242
N	-0.46812210	-1.68900581	-0.08747516
Te	-5.15604481	0.77451358	0.29469081
H	-1.45521297	-3.60224601	-0.14547642

S_{2T}

C	-2.36343602	-0.57084319	0.16031523
C	-0.93777593	-0.41241646	-0.00466605
C	-1.01358596	1.81485457	0.08433739
C	-3.11920535	0.58145987	0.33811278
C	-1.56290691	-2.54097851	-0.05819013
H	-2.84662176	2.62968226	0.49889912

H	0.49553009	-1.95187809	-0.27838644
N	-2.36155894	1.77037880	0.26803201
N	-0.41925493	3.06796048	0.08725161
H	0.54593683	3.00378092	-0.21345540
H	-0.91931071	3.76828196	-0.45059347
N	-0.23934704	0.72096432	-0.06932526
N	-2.71176867	-1.90838604	0.10773336
N	-0.46636774	-1.68994038	-0.12660918
Te	-5.16388000	0.83474240	-0.19964198
H	-1.44653051	-3.61134237	-0.14457884

S_{1T}

C	-2.35110209	-0.54956985	0.12170233
C	-0.97003375	-0.41139116	-0.01925439
C	-0.99682851	1.80936610	0.03937288
C	-3.12922123	0.60755516	0.28369010
C	-1.57550852	-2.53145276	-0.05667015
H	-2.76611896	2.64611906	0.56647559
H	0.47581284	-1.95124553	-0.24600035
N	-2.36782381	1.80531282	0.16892611
N	-0.42241060	3.07462097	0.10503425
H	0.56508706	3.02048986	-0.11447354
H	-0.88332986	3.75592630	-0.48757934
N	-0.23797650	0.75089873	-0.09156199
N	-2.72199290	-1.87642525	0.09111219
N	-0.49027461	-1.68983991	-0.12483360
Te	-5.18822171	0.65059402	-0.11831870
H	-1.47014036	-3.60463801	-0.11838669

T_{2T}

C	-2.34526389	-0.54809403	0.16359194
C	-0.97232074	-0.40986377	-0.01325107
C	-0.99891499	1.80543492	0.04878454
C	-3.13231479	0.60756023	0.36887037
C	-1.57921499	-2.52937061	-0.04997839
H	-2.75980239	2.64978822	0.59054446
H	0.46707491	-1.94336323	-0.29787626
N	-2.35892079	1.79235225	0.23322499
N	-0.42160134	3.06932010	0.09453473
H	0.55440278	3.01418849	-0.17155825
H	-0.90899792	3.75948992	-0.46569234
N	-0.23924232	0.74777234	-0.10141780
N	-2.71839318	-1.87372738	0.13431020
N	-0.49503396	-1.68584825	-0.14058984
Te	-5.14560271	0.65301605	-0.27086539
H	-1.47593722	-3.60233473	-0.12339716

T_{1T}

C	-2.36193616	-0.56044946	0.17408225
C	-0.97546951	-0.41156174	-0.02956373
C	-1.00753151	1.80582927	0.06613723
C	-3.14713610	0.60084611	0.39982846
C	-1.56894249	-2.53237432	-0.03807605
H	-2.80018894	2.65912128	0.48366595
H	0.47122215	-1.93485588	-0.31725910
N	-2.34603506	1.78306823	0.26273974

N	-0.39802588	3.04824064	0.09678807
H	0.54947599	2.99366600	-0.25540818
H	-0.92266938	3.79304531	-0.34435886
N	-0.24459676	0.73410116	-0.09821163
N	-2.71114721	-1.89093907	0.16054604
N	-0.49171384	-1.68393126	-0.15358060
Te	-5.11681758	0.70778150	-0.29972515
H	-1.45857124	-3.60526723	-0.10836967

S_{2P}

C	-2.36178791	-0.56617830	0.01842783
C	-0.94808694	-0.41989537	-0.02789288
C	-1.00751990	1.80824613	0.04364620
C	-3.12473714	0.58639720	0.07719721
C	-1.55153023	-2.53818615	-0.07603858
H	-2.88229766	2.64745096	0.25526651
H	0.51025161	-1.95583590	-0.13686111
N	-2.36935003	1.78520303	0.10531767
N	-0.40278319	3.04486948	0.13945308
H	0.58164289	2.99459246	-0.08972514
H	-0.87229827	3.79729858	-0.34773462
N	-0.24406596	0.73052626	-0.03587623
N	-2.71095040	-1.90325643	-0.01007282
N	-0.46249515	-1.69145871	-0.09078191
Te	-5.25329876	0.79778654	0.29098287
H	-1.43077654	-3.61123927	-0.11607334

S_{1P}

C	-2.35853089	-0.55108256	-0.00845578
C	-0.97295147	-0.41190710	-0.04172268
C	-0.99683885	1.81077768	0.02091673
C	-3.14431873	0.61655945	-0.01046927
C	-1.56641652	-2.53319662	-0.06276296
H	-2.79980704	2.63550880	0.49718032
H	0.48949416	-1.95515319	-0.11599044
N	-2.37386590	1.81060963	0.09738766
N	-0.42684203	3.07625878	0.13579241
H	0.57433278	3.01947301	-0.01028334
H	-0.84087811	3.75651734	-0.49176446
N	-0.24070207	0.75384116	-0.08972682
N	-2.72303008	-1.88017805	-0.02093206
N	-0.48342344	-1.69292370	-0.08103468
Te	-5.21022499	0.65886889	0.26034893
H	-1.45608041	-3.60765300	-0.07924883

T_{2P}

C	-2.35634120	-0.55607985	0.01726855
C	-0.97336936	-0.41343705	-0.03430209
C	-0.99827610	1.80386464	0.05889757
C	-3.15206377	0.60784203	0.01853138
C	-1.56144366	-2.53711059	-0.07354865
H	-2.80869679	2.66036406	0.35522011
H	0.49173953	-1.94776010	-0.14505502
N	-2.36370242	1.78802504	0.11654738
N	-0.43773375	3.07583281	0.15207907
H	0.56211429	3.01591872	-0.00012815

H	-0.85216950	3.73905098	-0.49391733
N	-0.23194183	0.75072850	-0.05359618
N	-2.71633799	-1.88443021	-0.00473672
N	-0.48214585	-1.69188265	-0.09516191
Te	-5.20203126	0.70601129	0.28943260
H	-1.44768391	-3.61061709	-0.10829586

T_{1P}

C	-2.37071564	-0.57030402	0.02348285
C	-0.96837082	-0.41985530	-0.02032269
C	-1.01178773	1.80939834	0.04780367
C	-3.14394123	0.59295736	0.10004246
C	-1.55289815	-2.54510910	-0.08385603
H	-2.85867730	2.65093641	0.24219003
H	0.50136588	-1.94145685	-0.13785688
N	-2.35701574	1.78421730	0.10893779
N	-0.41467016	3.05727087	0.14802084
H	0.57141627	3.00020039	-0.07371037
H	-0.87188099	3.78439972	-0.38838943
N	-0.23589260	0.73496751	-0.02078223
N	-2.71639491	-1.89919082	-0.01501034
N	-0.47432010	-1.69048023	-0.09098562
Te	-5.19438286	0.77541344	0.29010212
H	-1.43191751	-3.61704451	-0.13043144

$(S_2/S_1)_T$

C	-2.34362276	-0.56708091	0.35848454
C	-0.95517777	-0.40521329	-0.04735560

C	-1.02879165	1.80375151	0.11830553
C	-3.08390399	0.56360369	0.68883392
C	-1.57959908	-2.52983403	0.00152852
H	-2.84743530	2.58576972	0.56477013
H	0.40828170	-1.91893663	-0.60237223
N	-2.30846362	1.72750647	0.48049395
N	-0.42865254	3.02768272	0.02019821
H	0.41672505	3.02701395	-0.53296642
H	-1.02696505	3.82840223	-0.12444604
N	-0.27310449	0.71381015	-0.15700276
N	-2.67117658	-1.91384815	0.38081941
N	-0.51182115	-1.66441625	-0.27272644
Te	-4.82754547	0.82590927	-0.76139202
H	-1.46883077	-3.59779996	-0.11593799

$(S_2/S_1/T_2)_P$

C	-2.38876576	-0.56292390	-0.09203005
C	-0.94733132	-0.37309519	-0.16219518
C	-1.09998298	1.87934025	-0.31103346
C	-3.13200187	0.59250838	0.14741637
C	-1.55500601	-2.51811551	-0.06793681
H	-2.92147460	2.60814590	0.33740660
H	0.51318093	-1.92349557	-0.18266507
N	-2.43637711	1.75088384	0.09632653
N	-0.57730654	3.16889170	-0.03404130
H	0.00621113	3.14653044	0.80518513
H	0.02725210	3.46677210	-0.79344633
N	-0.26882986	0.73646958	-0.22055491

N	-2.71634258	-1.90555277	-0.04053147
N	-0.45845518	-1.66298392	-0.11745401
Te	-5.14830063	0.69361369	0.69059286
H	-1.42655319	-3.59066845	-0.05580417

$(S_1/T_2/T_1)_P$

C	-2.36578639	-0.55525643	0.08718266
C	-0.92506404	-0.39534920	-0.01629288
C	-1.01555568	1.83869745	0.11188001
C	-3.12783169	0.59680736	0.20182300
C	-1.56859626	-2.52100997	-0.10444352
H	-2.89179884	2.63390701	0.44266806
H	0.50422418	-1.96942350	-0.23874092
N	-2.40603788	1.77787222	0.20646328
N	-0.49395296	3.14448178	0.06711892
H	0.50811859	3.10244623	0.22566283
H	-0.63675020	3.57739676	-0.84779381
N	-0.24419876	0.73326781	-0.03486055
N	-2.71775342	-1.89044739	0.01833475
N	-0.45741079	-1.69229247	-0.12270828
Te	-5.22697723	0.71933091	0.18510141
H	-1.46471212	-3.59410805	-0.18216028

$(S_1/T_2/T_1)_T$

C	-2.34508239	-0.55109301	0.13933301
C	-0.99021965	-0.41248286	-0.04915512
C	-0.98493303	1.78992227	0.06499521
C	-3.12085756	0.60842052	0.39216078

C	-1.56123847	-2.51708146	-0.04135259
H	-2.74027246	2.62268203	0.58869820
H	0.46216604	-1.93144192	-0.27982171
N	-2.33274815	1.77847804	0.26558745
N	-0.41561332	3.04786910	0.08250905
H	0.54326335	3.02064635	-0.18375048
H	-0.92131177	3.72613826	-0.44272816
N	-0.26509780	0.75273736	-0.11543627
N	-2.67929679	-1.89630411	0.13375038
N	-0.48685892	-1.68073383	-0.15739311
Te	-5.23697479	0.72825638	-0.30448663
H	-1.45500783	-3.57969262	-0.09367527

$(T_1/S_0)_T$

C	0.40556039	-0.83424791	0.24583788
C	1.72214063	-0.39803160	-0.01443787
C	1.24919933	1.75256623	0.14601030
C	-0.63571852	0.14260726	0.51166920
C	1.59480012	-2.60137887	0.05873986
H	-0.65300545	2.21543995	0.64052407
H	3.45367855	-1.58168297	-0.30799529
N	-0.03598264	1.44210808	0.43796978
N	1.58574643	3.09290187	0.17895359
H	2.49788339	3.25722076	-0.22672481
H	0.88382196	3.73079253	-0.17178268
N	2.20383688	0.86853124	-0.09640702
N	0.35544954	-2.21676633	0.28662465
N	2.46278755	-1.53959862	-0.12180880

Te	-1.94831284	-0.22468900	-1.21620462
H	1.93640085	-3.62439143	0.00849183

TeC

S_0

C	0.32305048	0.63249821	-0.13768246
C	2.34673419	1.76212501	-0.05472281
C	1.71562446	3.03700114	0.11937552
C	0.35427396	3.04089714	0.10345318
H	2.28162538	3.95191965	0.23376171
H	-0.24385365	3.93887381	0.20865585
H	-1.33489249	1.84527125	-0.03994732
N	3.69875359	1.68477903	-0.13207661
H	4.26589541	2.45325607	0.18380209
H	4.09919253	0.75881642	-0.10199224
N	1.67171379	0.62220389	-0.17544281
N	-0.32211378	1.87549716	-0.05045143
Te	-0.85050792	-1.03742573	-0.16083542

S_{2P}

C	0.36997554	0.68967006	-0.13139886
C	2.36837730	1.82993847	-0.08474362
C	1.72591253	3.03423680	0.06401883
C	0.32197092	3.08244480	0.11737817
H	2.28923730	3.95823761	0.13517480
H	-0.28768956	3.96448523	0.23657302
H	-1.34366085	1.78600636	0.05428784
N	3.74597798	1.67206308	-0.23286866
H	4.29313635	2.39310139	0.21865315
H	4.03795665	0.74876093	0.06508546
N	1.66690523	0.60360932	-0.19006396

N	-0.33638560	1.84784079	0.01477377
Te	-0.84621784	-1.04468179	-0.27097273

S_{2T}

C	-0.55745277	0.36033650	0.28827193
C	1.18977492	1.86829652	0.07486491
C	2.16783830	0.84024975	0.12912505
C	1.72324586	-0.44796681	0.30647753
H	3.22552230	1.04918735	0.03447083
H	2.37561406	-1.31336657	0.32000984
H	0.02380175	-1.61603497	0.50071389
N	1.56234413	3.19483637	0.05666275
H	2.45520076	3.40449297	-0.36550665
H	0.81342613	3.80633050	-0.24287035
N	-0.12655379	1.61757602	0.09932891
N	0.39243072	-0.67775756	0.40788512
Te	-2.18017813	-0.29703124	-1.05342347

S_{1P}

C	0.34563502	0.70628445	-0.11140583
C	2.35756337	1.81349515	-0.08601309
C	1.71021702	3.03645229	0.06052195
C	0.33079089	3.09559780	0.14121823
H	2.28185614	3.95766730	0.10737730
H	-0.25614200	3.98929119	0.29391364
H	-1.35434577	1.86289034	-0.13685214
N	3.74452686	1.67106928	-0.25592479
H	4.27496676	2.34317105	0.28627974

H	4.02851235	0.73051417	-0.00497995
N	1.63426835	0.62122653	-0.18808775
N	-0.37707082	1.85892550	0.11564526
Te	-0.71528225	-1.12087199	-0.22579532

S_{1T}

C	-0.54544573	0.32633708	0.12692214
C	1.16874140	1.86890743	0.05614223
C	2.17112819	0.82505341	0.09994538
C	1.73941899	-0.44918842	0.27932292
H	3.22627490	1.04330210	-0.00534323
H	2.40453919	-1.30427940	0.33310640
H	0.05782525	-1.61571572	0.68819227
N	1.56533851	3.20367652	0.13764885
H	2.43111994	3.40333459	-0.34869572
H	0.82264269	3.82368352	-0.16767505
N	-0.12085957	1.59406365	-0.02776736
N	0.39018409	-0.70075806	0.42323397
Te	-2.24589361	-0.22926786	-1.03902251

T_{2P}

C	0.36000102	0.70236539	-0.11915242
C	2.35888774	1.81238933	-0.07212401
C	1.70019170	3.05189732	0.03007082
C	0.32807783	3.10182950	0.10695669
H	2.27463045	3.97302592	0.03196787
H	-0.27169603	3.99133416	0.22570469
H	-1.35941445	1.84157058	0.04227994

N	3.74856413	1.68702931	-0.21231474
H	4.27121345	2.30298291	0.39972218
H	4.02907009	0.72494822	-0.05516547
N	1.63693407	0.61997246	-0.21190703
N	-0.35676092	1.86046248	0.13918643
Te	-0.71420314	-1.10409454	-0.30932770

T_{2T}

C	-0.56976154	0.32288040	0.23974582
C	1.15786431	1.86203877	0.05859527
C	2.16769774	0.83201696	0.09509452
C	1.73393684	-0.44166054	0.27786581
H	3.22141464	1.05616003	-0.00388074
H	2.39760407	-1.29665190	0.34498108
H	0.08013975	-1.62491935	0.61490676
N	1.55660085	3.18168903	0.07391814
H	2.45816510	3.38147628	-0.33329601
H	0.82761983	3.82678910	-0.20109167
N	-0.13141788	1.60220310	0.05061672
N	0.40164472	-0.68487991	0.43634822
Te	-2.23649418	-0.22799315	-1.09779364

T_{1P}

C	0.36463596	0.69906178	-0.16351501
C	2.36623106	1.83337193	-0.09087405
C	1.70604243	3.04956756	0.04627354
C	0.32119761	3.09759809	0.10417429
H	2.27478694	3.97410202	0.07828098

H	-0.27940605	3.99510662	0.14893182
H	-1.35408521	1.79054515	0.17129164
N	3.76556613	1.72593003	-0.19900138
H	4.26050453	2.22885353	0.53099617
H	4.03851375	0.75001847	-0.17118206
N	1.66108213	0.63926321	-0.25533155
N	-0.36049879	1.86030693	0.00980726
Te	-0.75907457	-1.07801228	-0.21395444

T_{1T}

C	-0.58951594	0.35801079	0.26607254
C	1.16192297	1.87853312	0.08314907
C	2.16054414	0.83750161	0.11117545
C	1.71315652	-0.43768072	0.27412125
H	3.21658358	1.05111948	0.01648838
H	2.36711143	-1.30121144	0.32477260
H	0.04136722	-1.61055362	0.56282926
N	1.58366588	3.19534452	0.08348008
H	2.45863816	3.36916505	-0.39102033
H	0.84895546	3.83609452	-0.18948960
N	-0.12882158	1.63737403	0.08822873
N	0.38171936	-0.67231841	0.39949453
Te	-2.15031296	-0.35223009	-1.07329167

T_{3P}

C	0.33214378	0.68059062	-0.18493777
C	2.35558401	1.77396329	-0.08468416
C	1.72622646	3.03418821	0.06558806

C	0.33042655	3.06141535	0.12309450
H	2.30094046	3.95079069	0.11572642
H	-0.27280347	3.95173461	0.23803173
H	-1.35228249	1.86244282	0.04309212
N	3.73005457	1.69150430	-0.19871117
H	4.24215266	2.39726563	0.30959671
H	4.07205479	0.75319592	-0.03779046
N	1.68455302	0.60983090	-0.18873189
N	-0.34503941	1.87480659	0.00769843
Te	-0.79851015	-1.07600903	-0.21207522

$(S_2/S_1/T_3/T_2/T_1)_P$

C	0.34308133	0.66982621	-0.15381259
C	2.35980332	1.78043319	-0.06062958
C	1.72230191	3.03622851	0.09188642
C	0.32055334	3.06291567	0.10847901
H	2.28583345	3.95596096	0.17955395
H	-0.28185464	3.95319255	0.22061739
H	-1.35362278	1.83272445	0.01473604
N	3.73349383	1.67922606	-0.16428841
H	4.29356335	2.42550749	0.21415965
H	4.09995513	0.74640533	-0.05219315
N	1.68243702	0.60502616	-0.17174013
N	-0.34562410	1.86971535	-0.02329731
Te	-0.85442036	-1.05144203	-0.20757400

$(S_2/S_1/T_2/T_1)_P$

C	0.38071943	0.69921298	-0.13244956

C	2.36669856	1.83973094	-0.08427609
C	1.73178237	3.03484309	0.06259827
C	0.32166417	3.07249157	0.11755387
H	2.28576322	3.95227010	0.12955474
H	-0.27412729	3.94942146	0.23852107
H	-1.32089669	1.79810010	0.05719069
N	3.74647568	1.67328003	-0.23085237
H	4.28494760	2.38270393	0.21507529
H	4.03701660	0.76863822	0.07209047
N	1.65002190	0.62596639	-0.18725805
N	-0.33261651	1.84931220	0.01575348
Te	-0.87195313	-1.08025796	-0.27760461

$(S_2/S_1/T_2)_T$

C	-0.55155696	0.36982138	0.41374080
C	1.21167783	1.85161261	0.08477653
C	2.15825888	0.84228195	0.13191699
C	1.71057596	-0.45871665	0.33870849
H	3.21632844	1.04120290	0.00800790
H	2.34746708	-1.33533029	0.30298557
H	-0.02117272	-1.59133150	0.42837733
N	1.54504759	3.17754308	0.00618200
H	2.43091194	3.42006670	-0.40706619
H	0.76351890	3.76099168	-0.26100413
N	-0.13000828	1.61845477	0.19997479
N	0.39583173	-0.66386090	0.42704075
Te	-2.01186614	-0.24358690	-1.11763054

$(T_2/T_1/S_0)_T$

C	-0.59862453	0.35969531	0.51144949
C	1.17381370	1.85540694	0.09992154
C	2.15989027	0.82693320	0.05406546
C	1.71357417	-0.44634180	0.29393033
H	3.20409273	1.02765848	-0.14391131
H	2.36066074	-1.31698647	0.27995098
H	0.06957342	-1.58839119	0.69912742
N	1.56230388	3.16936777	0.04055416
H	2.43801684	3.37412740	-0.41552376
H	0.80936012	3.81248609	-0.16403004
N	-0.13136072	1.61717592	0.25395664
N	0.40534324	-0.64277953	0.57809499
Te	-2.10162962	-0.25920327	-1.53157560