Sulfur reactions and photodissociations for Titan:

This chemical scheme for sulfur species has been used in the following paper:
K.M. Hickson, J.C. Loison, T. Cavalié, E. Hébrard, and M. Dobrijevic. The evolution of infalling sulfur species in Titan's atmosphere. Astronomy and Astrophysics. 2014.

See KIDA for the nomenclature of rate constants and uncertainties (See http:// kida.obs.u-bordeaux1.fr/help).

Reaction		ΔH_r(298K) kJ/mol	α	β	γ	F_0	g	references
H + SH	→ H_2 + S	-79	3.0e-11	0	0	5	0	(Cupitt & Glass 1975, Peng *et al.* 1999)
H + H_2S	→ H_2 + SH		3.66e-12	1.94	455	1.6	100	(Peng *et al.* 1999)
H + CS	→ HCS		k_0=7.5e-34 k_∞=1.0e-10	0.2 0	0 800	3 3	0 100	/ H + CO, barrier calculated at M06-2X/cc-pVTZ
H + HCS	→ H_2 + CS		1.0e-10	0	0	2	0	/ H + HCO and also (Galland *et al.* 2001)
H + H_2CS	→ HCS + H_2		3.3e-11	0	1400	3	200	/ H + H_2CO with smaller barrier
H + CH_3S	→ H_2CS + H_2 → CH_3 + SH	-210 -50	1.0e-11 3.0e-11	0 0	0 0	3 3	0 0	by comparison with CH_3O + H considering than the H_2CS + H_2 channel is much less exothermic than the corresponding H_2CO + H_2 (-210 compared to -344).
H + CH_3SH	→ CH_3S + H_2		7.8e-11	0	1310	1.8	200	(Amano *et al.* 1983)
^{2}H + ^{2}HCCS	→ H_2CCS → H_2 + CCS → $^3CH_2$ + CS	-373 -1.0 +102	k_0=2.0e-27 k_∞=1.0e-10 0 0	-1.5 0	0 0	3 3	0 0	M06-2X/cc-pVTZ / Semi empirical model
^{2}H + ^{2}CCS	→ HCCS → C_2H + S → CH + CS	-425 +52 +106	k_0=1.0e-27 k_∞=1.0e-10 0 0	-1.5 0	0 0	3 3	0 0	M06-2X/cc-pVTZ / Semi empirical model
H + CH_3CS	→ HCS + CH_3 → H_2 + H_2CCS		4.0e-11 2.0e-11	0 0	0 0	3 3	0 0	/ H + CH_3CO
H + CH_3CHS	→ H_2 + CH_3CS	-17	2.23e-11	0	1200	3	200	/ H + CH_3CHO with smaller E#
H + C_3S	→ HC_3S		k_0=3.0e-25	-2.93	176	10	0	Equal to H + C_4H_2

		k_∞=1.0e-10	0	800	3	100	Equal to H + CS
H + HC_3S	→ H_2 + C_3S	-118	2.0e-11	0	0	3	0	Energy calculated at M06-2X/cc-pVTZ, the main exit channel may be H_2C_3S formation.
	→ C_2H_2 + CS	-177	2.0e-11	0	0	3	0	
H + C_2H_2S	→ C_2H_2 + SH		2.87e-11	0	946	3	100	/ by comparison with C_2H_4S + H
H + C_2H_4S	→ C_2H_4 + SH		2.87e-11	0	946	1.8	100	(Lee *et al.* 1977a)
H + OCS	→ SH + CO		9.06e-12	0	1940	2	200	(Lee *et al.* 1977b, Rice *et al.* 1993a, Tsunashima *et al.* 1975, Adriaens *et al.* 2010)
H + N_2S	→ N_2 + SH	-270	2.1e-10	0	2600	1.6	100	M06-MP2/cc-pVTZ calculations
H + NCS	→ HCN + S	-93	0					
	→ HNC + S	-40	1.0e-10	0	0	2	0	submerged exit barrier on the triplet surface, need ISC as there is likely a barrier on the triplet entrance barrier but not on the entrance singlet surface by comparison with H + NCO (Klippenstein & Harding 2009))
C + H_2S	→ H + HCS	-178	2.1e-10	0	0	1.6	0	(Deeyamulla & Husain 2006, Galland et al. 2001)
C + OCS	→ CO + CS	-386	5.6e-11	0	0	2	0	(Loison *et al.* 2012b, Deeyamulla & Husain 2006, Deeyamulla & Husain 2007)
C + CS_2	→ CS + CS	-242	1.6e-10	0	0	3	0	(Deeyamulla & Husain 2006)
^{2}CH + ^{1}CS	→ ^{2}H + ^3C_2S	-106	1.5e-10	0	0	2	0	Very likely no barrier
	→ ^{3}S + ^2C_2H	-54	5.0e-11	0	0	2	0	
^{2}CH + ^1H_2S	→ ^{2}H + ^1H_2CS	-239	2.0e-10	0	0	2	0	By comparison with CH + H_2O (Bergeat *et al.* 2009, Hickson *et al.* 2013)
^{2}CH + ^{1}OCS	→ ^{2}HCS + ^{1}CO	-268	4.0e-10	0	0	2	0	(Loison *et al.* 2012b)
	→ ^{2}H +^{1}CS + ^{1}CO	-57	0					
^{2}CH + $^1CS_2$	→ ^{2}HCS + ^{1}CS	-124	4.0e-10	0	0	2	0	Considering the high CH reactivity and the stability of HCS
CH + N_2S	→ N_2 + HCS	-497	1.5e-11	0	-257	2	0	/CH + N_2O (Becker *et al.* 1993)
	→ HCN + NS	-364	1.5e-11	0	-257	2	0	
$^1CH_2$ + CS	→ HCCS + H	-158	2.0e-10	0	0	2	0	Very likely no barrier
$^3CH_2$ + CS	→ HCCS + H	-102	6.0e-11	0	0	2	0	no barrier at M06-2X/cc-pVTZ and also at MP2/cc-pVTZ level
CH_2 + CCS	→ HC_3S + H		1.0e-10	0	0	3	0	/ CH_2 + CH_3

CH_2 + HCCS	→ H_2C_3S + H	-179	1.0e-10	0	0	3	0	/ CH_2 + CH_3
$^3CH_2$ + C_3S	→ l-C_3H_2 + CS → HC_4S + H	-108 -186	6.0e-11 0	0	0	2	0	Assuming no barrier / $^3CH_2$ + CS. HC_4S very likely the main product but should react with H (and also to CH_3) to give C_3H_2 + CS. We avoid introducing new minor species.
CH_2 + NS	→ H + HCNS(=HNCS)	-193	1.0e-10	0	0	3	0	/ CH_2 + NO at 150K
CH_3 + CS	→ H_2CCS + H	-30	2.0e-12	0	2400	3	400	Average between M06-2X and MP2 /cc-pVTZ
CH_3 + SH	→ CH_3SH → H_2CS + H_2 → HCSH + H_2 → CH_2SH + H → CH_3S + H → $^1CH_2$ + H_2S → CH_4 + S	-308 -160 +27 +86 +50 +122 -82	k_0=1.0e-28 k_∞=1.2e-10 0 0 0 0 0 0	-3.5 0	0 0	3 3	0 0	M06-2X/cc-pVTZ/semi empirical model TS(→ H_2CS + H_2) very likely > 0 TS(→ HCSH + H_2) : +81 kJ/mol
CH_3 + HCS	→ CH_4 + CS		9.3e-11	0	0	2	0	/ CH_3 + HCO. We neglect the association reaction as CH_3CHS absorbs strongly in the 190-230 nm (Rosengren 1962) and dissociate leading very likely to HCS, CS and CH_3CS all leading to CS formation.
CH_3 + C_2S	→ H + H_2C_3S → C_2H_3 + CS	-159 -126	2.0e-11 2.0e-11	0 0	0 0	3 3	0 0	the TS from $^2CH_3CCS$ toward $^2CH_2CHCS$ is found -218 kJ/mol below the entrance level followed by a small barrier equal to 6.7 kJ/mol above the exit channel for H elimination, and there is no exit TS at M06 and MP2 level for the $^2C_2H_3$ + ^{1}CS production
CH_3 + HCCS	→ C_2H_4 + CS	-151	2.0e-11	0	0	3	0	See text
CH_3 + NS	→ H + H_2CNS → H_3CNS (SOOT)	+21	0 k_0=1.1e-29 k_∞=1.1e-11	 -3.5 0.60	 0 0	 2 1.6	 0 0	/ CH_3 + NO
C_2 + H_2S	→ C_2H + HS	-226	2.0e-10	0	0	2	0	(Kaiser *et al.* 2002, Wang *et al.* 2003)
C_2 + CS_2	→ C_2S + CS	-198	2.0e-10	0	0	2	0	By comparison with $C_2(a^3\Pi_u)$ (Hu *et al.* 2014, Huang *et al.* 2004) reaction, the ground C_2 ($X^1\Sigma^+_g$) being more reactive (Canosa *et al.*

								2007, Daugey *et al.* 2008).
C_2 + OCS	→ C_2S + CO	-342	2.0e-10	0	0	2	0	By comparison with C_2 + CS_2
^2C_2H + ^1CS	→ ^1C_3S + ^2H	-62	1.0e-10	0	0	2	0	/ C_2H + CO (Lander *et al.* 1990, Petrie 1996)
^2C_2H + ^1H_2S	→ $^1C_2H_2$ + ^2HS	-172	1.0e-10	0	0	3	0	No barrier for preliminary DFT calculations
^2C_2H + $^1CS_2$	→ HCCS + CS	-25	6.0e-11	0	0	6	0	No barrier in the entrance valley at M06-2X/cc-pVTZ level but may be a small one in the exit valley.
^2C_2H + ^1OCS	→ HCCS + CO	-169	4.0e-11	0	0	5	0	Likely no barrier
^2C_2H + ^1C_3S	→ products		1.0e-10	0	0	3	0	/ C_2H + CO (Lander *et al.* 1990, Petrie 1996)
C_2H_3 + HS	→ C_2H_2 + H_2S → H_2C_2 + H_2S → H_2CCSH + H → HSCCH + H_2	-222 -30 +83 -177	5.0e-11 0 0 0	0	0	2	0	C_2H_3 + OH (Tsang & Hampson 1986) HSCCH likely a minor product by comparison with C_2H_3CN photodissociation (<<50%) neglected here.
C_2H_3 + CS	→ H_2C_3S + H	-33	3.0e-11	0	0	3	0	no barrier at M06-2X and MP2 level /cc-pVTZ
C_2H_3 + C_3S	→ H_2C_5S + H	-97	3.0e-11	0	0	3	0	Equal to C_2H_3 + CS
CN + H_2S	→ HCN + HS	-165	2.0e-10	0	0	2	0	Very likely no barrier as H_2S is much more reactive than H_2O
CN + CS_2	→ NCS + CS	+8	0					
CN + OCS	→ NCS + CO	-136	1.0e-10	0	0	3	0	(Loison et al. 2012b)
O + CS	→ S + CO		2.61e-10	0	758	2	100	(Lilenfeld & Richardson 1977)
OH + CS	→ H + OCS → CO + HS		1.7e-10 3.0e-11	0 0	0 0	3 3	0 0	(Rice & Chabalowski 1994, Loison *et al.* 2012a)
S + CH_3	→ H_2CS + H → H_2 + CS + H	-87 +93	1.4e-10 0	0	0	3	0	by comparison with O + CH_3
S + C_2H_2	→ C_2H_2S		k_∞ = 1.4e-11 k_0 = 5.5e-30	0 0	1010 0	1.8 10	200 0	(Strausz *et al.* 1971, Little & Donovan 1973) = k_0(OH + C_2H_2)
S + C_2H_3	→ SH + C_2H_2 → H + H_2C_2S	-199 -161	1.0e-11 6.0e-11	0 0	0 0	2 2	0 0	By comparison with O + C_2H_3 (Heinemann *et al.* 1988, Harding *et al.* 2005)
S + C_2H_4	→ C_2H_4S		k_∞ = 7.14e-12 k_0 = 1.0e-28	0 0	795 0	1.8 10	200 0	(Davis *et al.* 1972) / OH + C_2H_4
S + CO	→ OCS		0					(Loison *et al.* 2012b)

S + NH	→ NS + H	-116	6.6e-11	0	0	2	0	/ O + NH
$S(^1D) + N_2$	→ $S(^3P) + N_2$	-111	8.5e-11	0	0	1.6	0	(Black & Jusinski 1985)
$S(^1D) + H_2$	→ SH + H	-27	2.1e-10	0	0	1.6	0	(Black & Jusinski 1985)
$S(^1D) + CH_4$	→ SH + CH_3 → H_3CS + H → $H_2CS + H_2$	-27 +20 -200	1.7e-10 0 0	0	0	2.0	0	(Black & Jusinski 1985)
SH + CO	→ HSCO		0					We neglect this reaction as there is a barrier in the entrance and the well is small (Rice *et al.* 1993b, Rice & Chabalowski 1994)
SH + CS	→ H + CS_2	-103	2.0e-10	0	0	3	0	/ OH + CS
$^2N + {}^1C_3S$	→ $^2CN + {}^3C_2S$ → $^2C_2N + {}^1CS$	-309 -355	2.0e-11 2.0e-11	0 0	0 0	3 3	0 0	/ $^2N + {}^1CO$ (Herron 1999)
$^2N + N_2S$	→ N_2 + NS		2.0e-11	0	0	3	0	$^2N + N_2O$ / (Herron 1999) with no barrier
$^2N + {}^1CS$	→ $^2CN + {}^3S$	-257	4.0e-11	0	0	3	0	/ $^2N + {}^1CO$ (Herron 1999)
$^4N + {}^2HCCS$	→ $^1HCN + {}^3CS$	-65	8.0e-11	0	0	3	0	/ N + CH_3
$^{2,4}N + {}^1SH$	→ $^2NS + {}^2H$	-94	4.5e-11	0	0	2	0	/ N + OH but NS is easily photodissociated
$^{2,4}N$ + NS	→ N_2 + S		4.0e-11	0	0	2	0	/ N + NO
$^{2,4}N$ + HCS	→ NH + CS → H + NCS → HCN + S	-114 -261 -354	2.0e-11 1.0e-11 4.0e-11	0 0 0	0 0 0	3 3 3	0 0 0	
NH_2 + CS	→ H + HNCS	-147	6.0e-11	0	0	3	0	No barrier at M06-2X/cc-pVTZ level and very likely also at MP2/cc-pVTZ level
NH + NS	→ N_2S + H → N_2 + SH		2.9e-11 1.2e-11	-0.30 -0.30	-77 -77	1.6 1.6	0 0	/ NH + NO / NH + NO
NH + CS	→ H + NCS → HNC + S	-147 -187	2.0e-11 4.0e-11	0 0	0 0	3 3	0 0	No barrier at M06-2X/cc-pVTZ level and at MP2/cc-pVTZ level
NS + NS	→ N_2S + S	-123	4.0e-11	0	0	3	0	No barrier

$CS_2 + h\nu$ → $^1CS + {}^3S$ → $^1CS + {}^1S$		>223 nm 0% 0%		<223 nm 40% 60%			http://satellite.mpic.de/spectral_atlas (Yang *et al.* 1980, Moltzen *et al.* 1988)
$OCS + h\nu$ → $^1CO + S(^1D)$		>291 nm 0%		<291 nm 100%			http://phidrates.space.swri.edu/
$H_2S + h\nu$ → $HS + H$ → $^3S + H_2$ → $S(^1D) + H_2$		>316 nm 0% 0% 0%	316-200 nm 100% 0% 0%	<200 nm 95% 3% 2%			http://phidrates.space.swri.edu/ (Feng *et al.* 1999, Watanabe & Jursa 1964, Hsu *et al.* 1992)
$CS + h\nu$ → $^3S + {}^3C$		>168 nm 0%		<168 nm 100%			
$HCS + h\nu$ → $H + CS$		>604 nm 0%		<604 nm 100%			EOM-CCSD. Some excited state may be not dissociative.
$H_2CS + h\nu$ → $H + HCS$ → $H_2 + CS$		>312 nm 0% 0%		<312 nm 100% 0%			(Judge *et al.* 1978) + EOM-CCSD
$CH_3SH + h\nu$ → $CH_3 + SH$ → $CH_3S + H$	306 356	> 334nm 0% 0%	334-222 nm 100% 0%	222-190 nm 100-(222-λ)/0.64 (222-λ)/0.64	< 190 nm 50% 50%		EOM-CCSD + (Steer & Knight 1968, Vaghjiani 1993) Absorption: http://phidrates.space.swri.edu/ but branching ratio from http://phidrates.space.swri.edu/ above 250 nm likely wrong. The selective S-H bond fission at 248 nm in CH_3SH photolysis is explained by assuming the Franck-Condon overlap between the ground vibrational wave function (at extended S-H geometries) and the dissociative surface to be on the CH_3S+H exit channel side only (Vaghjiani 1993).
$CH_3CHS + h\nu$ → $CH_3 + HCS$ → $CH_3CS + H$	359 376	>318 nm 0% 0%		<318 nm 100% 0%			We neglect the CH_3CS formation considering than H + CH_3CS give CH_3 + HCS.
		>274 nm		<274 nm			EOM-CCSD

$C_2S + h\nu$	$\rightarrow C + CS$ $\rightarrow C_2 + S$	436 647	0% 0%		100% 0%		
HCCS + hν	$\rightarrow H + CCS$ $\rightarrow C_2H + S$ $\rightarrow CH + CS$	425 477 531	>281 nm 0% 0% 0%	282-251 nm 100% 0% 0%	<251 nm 80% 20% 0%		EOM-CCSD
$H_2CCS + h\nu$	$\rightarrow H + HCCS$ $\rightarrow H_2 + HCCS$ $\rightarrow {}^3CH_2 + CS$ $\rightarrow {}^1CH_2 + CS$	375 372 475 513	>319 nm 0% 0% 0% 0%		<319 nm 100% 0% 0% 0%		EOM-CCSD
$C_3S + h\nu$	$\rightarrow C_2 + CS$ $\rightarrow C_3 + {}^3S$ $\rightarrow C_3 + {}^1S$ $\rightarrow C + C_2S$	655 519 669 699	>182 nm 0% 0% 0% 0%	182-179nm 100% 0% 0%	179-171nm 50% 0% 50% 0%	<171nm 40% 0% 40% 20%	EOM-CCSD
$H_2C_3S + h\nu$	$\rightarrow C_2H_2 + CS$ $\rightarrow H + HC_3S$ $\rightarrow H_2 + C_3S$	181 355 237	>290 nm 0% 0% 0%		<290 nm 30% 40% 30%		EOM-CCSD
$H_2C_5S + h\nu$	$\rightarrow C_4H_2 + CS$ $\rightarrow H + HC_5S$ $\rightarrow C_2H_2 + C_3S$ $\rightarrow H_2 + C_5S$		>290 nm 0% 0% 0% 0%		<290 nm 50% 0% 50% 0%		Same absorption than H_2C_3S. $H + HC_5S$ and $H_2 + C_5S$ very likely important channels but should give CS and C_3S through photodissociation and reactions with H atoms.
NS + hν	$\rightarrow N + S$	464	>258 nm 0%		<258 nm 100%		
$N_2S + h\nu$	$\rightarrow N_2 + S(^1D)$	187	>640 nm 0%		<640 nm 100%		EOM-CCSD
HNCS + hν	$\rightarrow H + NCS$ $\rightarrow HNC + S$	375 335	>320 nm 0% 0%		<320 nm 30% 70%		EOM-CCSD + (Boxall & Simons 1973)

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