

**Reactivity of hydropersulfides toward hydroxyl radical unraveled:
disulfide bond cleavage, hydrogen atom transfer, and proton-coupled
electron transfer**

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(Supplementary Information)

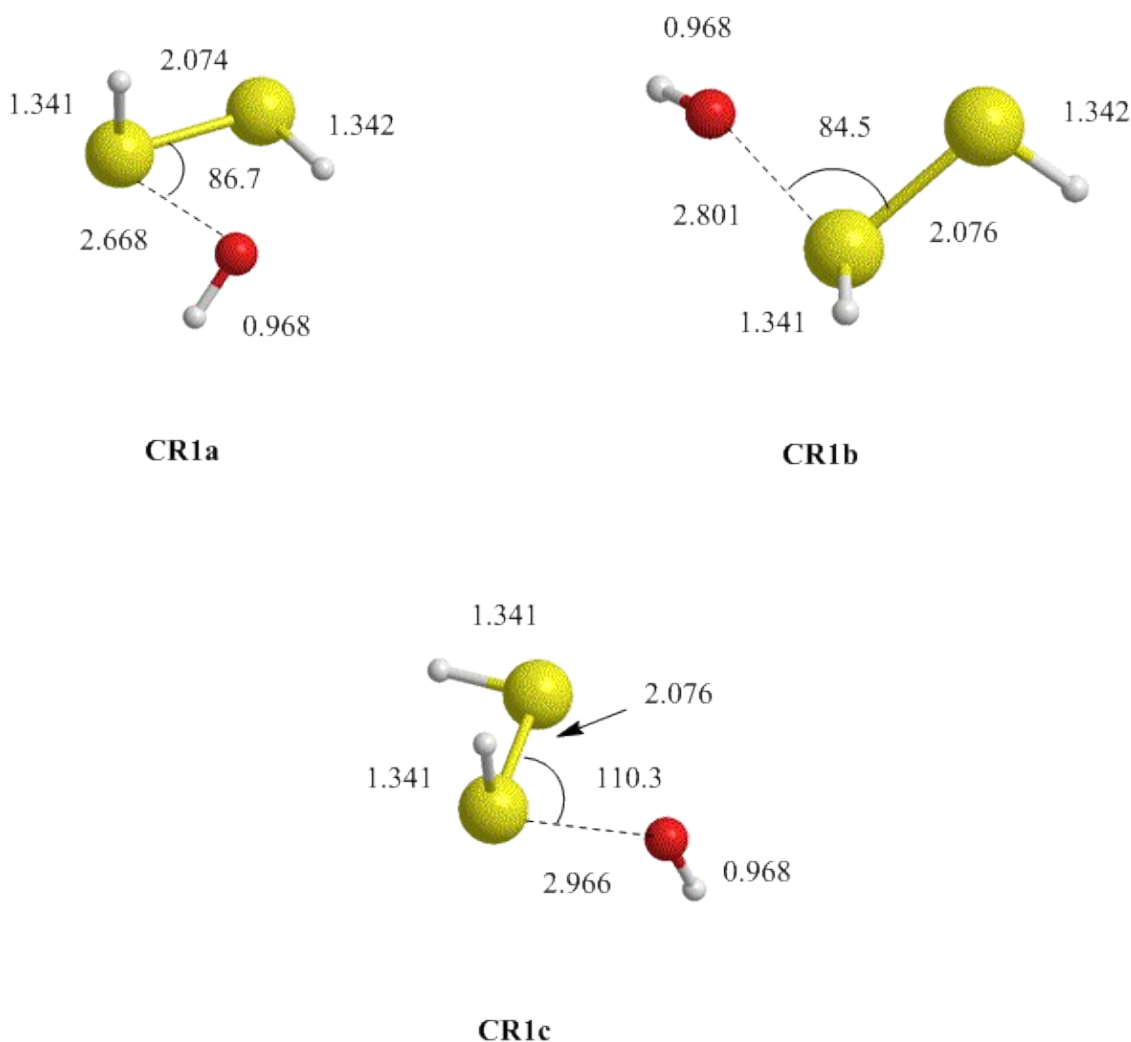


Figure S1: Main geometrical parameters (distances in Angstrom and angles in degree) of the pre-reactive complexes for the HSSH + OH reaction.

Table S1 : Relative energies ($\Delta(E+ZPE)$) and free energies ($\Delta G(298K)$), values in kcal·mol⁻¹, for the reaction between OH and RSSH, computed at CCSD(T)/aug-cc-pV(T+d)/QCISD/6-11+G(2df,2p) level of theory.

R =	H	CH₃	NH₂	COOH	CN	NO₂
HSSR + OH	0.00	0.00	0.00	0.00	0.00	0.00
RSSH + OH → HSOH + SR (Reaction 1)						
CRBTS1a	-2.13 (3.39)	-1.81 (3.88)	-2.65 (4.12)	-0.65 (4.83)	-2.74 (2.85)	-1.98 (3.54)
BTS1a	-1.51 (6.51)	-1.42 (6.65)	0.07 (8.01)	-0.02 (8.05)	-1.13 (6.91)	-0.01 (8.18)
CPBTS1a	-10.32 (2.25)	-9.07 (-1.24)	-19.60 (-13.13)	-9.17 (-1.47)	-14.64 (-8.76)	-7.59 (-0.08)
CRBTS1b	-2.94 (3.99)	-2.47 (3.99)	-1.47 (5.04)	-2.01 (3.43)	-4.23 (2.36)	-3.98 (2.74)
BTS1b	-1.76 (6.28)	-2.42 (5.75)	-1.46 (6.59)	-1.14 (6.85)	-1.60 (6.34)	-1.38 (6.88)
CPBTS1b	-9.82 (-1.87)	-8.44 (-0.50)	-19.62 (-13.18)	-11.21 (-3.19)	-14.64 (-8.76)	-10.88 (-3.11)
CRFTS1a	-2.94 (3.99)	-2.49 (3.86)	-2.67 (4.05)	-5.20 (1.60)	-4.15 (2.68)	-4.06 (3.71)
FTS1a	6.27 (14.56)	8.11 (16.47)	6.85 (15.59)	8.44 (17.28)	6.93 (14.98)	10.95 (19.47)
CPFTS1a	-8.55 (-2.39)	-9.04 (-3.60)	-19.35 (-13.32)	-15.86 (-7.87)	-14.64 (-8.76)	-7.61 (-0.11)
CRFTS1b	-1.89 (4.22)	-1.79 (3.89)	-1.47 (5.04)	-1.86 (4.37)	-2.22 (4.68)	-0.04 (6.61)
FTS1b	4.44 (12.75)	4.44 (12.73)	3.26 (11.75)	4.22 (12.66)	2.06 (10.64)	5.48 (14.01)
CPFTS1b	-8.55 (-2.39)	-10.88 (-5.30)	-22.31 (-15.42)	-11.01 (-3.39)	-14.60 (-8.54)	-7.59 (-0.12)
HSOH + SR	-6.43 (-6.56)	-5.69 (-7.66)	-15.11 (-17.20)	-5.38 (-7.79)	-11.80 (-12.65)	-2.20 (-4.70)
RSSH + OH → RSOH + SH (Reaction 2)						
CRBTS2a	-2.13 (3.39)	-5.38 (1.97)	-5.43 (1.97)	-2.15 (4.38)	-4.12 (2.24)	-1.49 (4.80)
BTS2a	-1.51 (6.51)	-4.49 (3.88)	-3.22 (4.94)	1.62 (9.97)	1.03 (9.37)	2.01 (10.12)
CPBTS2a	-10.32 (2.25)	-13.64 (-5.79)	-18.12 (-10.54)	-10.42 (-4.85)	-11.23 (-5.22)	-10.88 (-5.44)
CRBTS2b	-2.94 (3.99)	-6.65 (1.13)	-6.45 (1.41)	--	-4.12 (2.24)	-1.66 (4.82)
BTS2b	-1.76 (6.28)	-5.63 (2.82)	-4.52 (3.81)	--	-0.25 (8.24)	0.97 (9.25)
CPBTS2b	-9.82 (-1.87)	-11.97 (-5.21)	-18.09 (-10.47)	--	-11.22 (-5.20)	-10.90 (-5.55)
CRFTS2a	-2.94 (3.99)	-6.64 (1.15)	-8.01 (0.03)	-3.17 (3.79)	-4.16 (2.64)	(a)
FTS2a	6.27 (14.56)	1.77 (10.21)	-0.60 (7.91)	6.09 (14.81)	5.86 (14.50)	(a)
CPFTS2a	-8.55	-11.97	-18.08	-15.03	-10.07	(a)

	(-2.39)	(-5.21)	(-10.45)	(-7.78)	(-5.53)	
CRFTS2b	-1.89	-5.39	-6.92	-2.14	-4.12	(a)
	(4.22)	(1.98)	(0.92)	(4.41)	(2.24)	
FTS2b	4.44	-0.34	-1.02	5.05	4.12	(a)
	(12.75)	(8.20)	(7.87)	(13.75)	(12.76)	
CPFTS2b	-8.55	-16.63	-21.28	-10.78	-10.12	(a)
	(-2.39)	(-8.55)	(-13.32)	(-5.27)	(-5.81)	
RSOH + SH	-6.43	-8.14	-13.17	-9.40	-8.44	-10.08
	(-6.56)	(-8.36)	(-13.39)	(-9.67)	(-8.68)	(-10.29)
RSSH + OH → SSR + H₂O (Reaction 3)						
CRHTS3a	-2.94	-6.66	8.00	-5.18	-4.16	-4.06
	(3.99)	(1.10)	(0.04)	(1.71)	(2.64)	(3.71)
HTS3a	-1.40	-2.18	-2.14	-1.78	-1.56	-1.84
	(5.82)	(5.20)	(5.21)	(5.73)	(5.95)	(5.65)
CPHTS3a	-45.37	-49.13	-51.03	-41.77	-45.07	-48.70
	(-40.26)	(-42.88)	(-44.08)	(-39.46)	(-38.97)	(-43.11)
CRHTS3b	2.13	-2.48	-3.35	-5.18	-4.16	-4.06
	(3.39)	(3.88)	(3.41)	(1.71)	(2.64)	(3.71)
HTS3b	-1.61	-2.07	-2.34	-3.65	-2.38	-3.81
	(5.64)	(5.19)	(4.92)	(3.91)	(5.17)	(4.18)
CPHTS3b	-47.07	49.13	-51.04	-41.77	-45.07	-48.70
	(-40.36)	(-42.88)	(-44.11)	(-39.46)	(-38.97)	(-43.11)
CRPTS3a	-2.94	-6.66	-6.44	--	--	--
	(3.99)	(1.10)	(1.44)			
PTS3a	2.53	-2.71	-1.63	--	--	--
	(10.54)	(6.09)	(7.07)			
CPPTS3a	-47.07	-49.13	-49.83	--	--	--
	(-40.36)	(-42.88)	(-42.95)			
CRPTS3b	--	-6.66	--	--	--	--
		(1.10)				
PTS3b	--	-0.55	--	--	--	--
		(7.84)				
CPPTS3b	--	-49.13	----	--	--	--
		(-42.88)				
NO₂SSH + OH → HSSOH + NO₂ (Reaction 10)						
CRFTS10b	--	--	--	--	--	-3.20
						(2.47)
FTS10b	--	--	--	--	--	0.85
						(9.19)
CPFTS10b	--	--	--	--	--	-36.38
						(-32.40)
CRFTS10a	--	--	--	--	--	-1.64
						(4.89)
FTS10a	--	--	--	--	--	0.32
						(8.56)
CPFTS10a	--	--	--	--	--	-35.37
						(-31.84)
CH₃SSH + OH → CH₂SSH + H₂O (Reaction 11)						
CRHTS11	-	-2.69	-	-	-	-

		(4.03)				
HTS11a	-	0.02	-	-	-	-
		(7.71)				
HTS11b	-	0.76	-	-	-	-
		(8.03)				
CPHTS11	-	-23.50	-	-	-	-
		(-18.92)				
CH₂SSH + H₂O	-	-21.72	-	-	-	-
		(-22.62)				
(COOH)SSH + OH → (COO)SSH + H₂O (Reaction 12)						
CRPTS12	-	-	-	-7.12	-	-
				(0.76)		
PTS12a	-	-	-	1.63	-	-
				(10.51)		
PTS12b	-	-	-	1.77	-	-
				(10.64)		
CPPTS12	-	-	-	-8.84	-	-
				(-3.88)		

a) Correspond to reaction 10

Table S2: Rate constants (in $M^{-1} \cdot s^{-1}$) at different temperatures (in kelvin), and branching ratios (Γ , in %).

OH + HSSH

T	k total	Kbackside	Kfrontside	Khat	Kpcet	$\Gamma_{\text{reaction2}}$	$\Gamma_{\text{reaction3}}$
220.00	1.09e+11	1.50e+10	3.24e+04	9.28e+10	1.31e+09	0.14	0.86
230.00	9.48e+10	1.27e+10	4.41e+04	8.10e+10	1.02e+09	0.13	0.87
240.00	8.36e+10	1.09e+10	5.86e+04	7.19e+10	8.21e+08	0.13	0.87
250.00	7.48e+10	9.48e+09	7.62e+04	6.46e+10	6.77e+08	0.13	0.87
260.00	5.76e+10	8.36e+09	9.75e+04	4.87e+10	5.71e+08	0.15	0.85
270.00	5.26e+10	7.46e+09	1.23e+05	4.47e+10	4.90e+08	0.14	0.86
280.00	4.85e+10	6.72e+09	1.52e+05	4.13e+10	4.29e+08	0.14	0.86
290.00	4.49e+10	6.11e+09	1.86e+05	3.84e+10	3.80e+08	0.14	0.86
298.00	3.59e+10	5.70e+09	2.17e+05	2.99e+10	3.49e+08	0.16	0.84
300.00	3.54e+10	5.60e+09	2.26e+05	2.94e+10	3.43e+08	0.16	0.84
310.00	3.33e+10	5.17e+09	2.70e+05	2.78e+10	3.12e+08	0.16	0.84
320.00	3.15e+10	4.82e+09	3.21e+05	2.64e+10	2.88e+08	0.15	0.85

OH + CH₃SSH

T	$\Gamma_{\text{reaction 1}}$	$\Gamma_{\text{reaction 2}}$	$\Gamma_{\text{reaction 9}}$	$\Gamma_{\text{reaction 3}}$
220.00	0.00	0.70	0.00	0.30
230.00	0.00	0.71	0.00	0.29
240.00	0.00	0.72	0.00	0.27
250.00	0.00	0.73	0.00	0.26
260.00	0.00	0.74	0.00	0.26
270.00	0.00	0.74	0.00	0.25
280.00	0.01	0.75	0.00	0.25
290.00	0.01	0.75	0.00	0.24
298.00	0.01	0.75	0.00	0.24
300.00	0.01	0.75	0.00	0.24
310.00	0.01	0.75	0.00	0.24
320.00	0.01	0.75	0.01	0.23

OH + CH₃SSH

T	K backs. react1	K fronts react 1	Kbacks react2	K fronts react2	K react9	K pcet react3	K hat react3
230.00	9.40e+10	2.21e+04	4.98e+13	3.58e+09	2.05e+10	1.97e+13	6.25e+11
240.00	7.72e+10	3.32e+04	3.03e+13	3.22e+09	1.90e+10	1.13e+13	5.22e+11

250.00	6.46e+10	4.87e+04	1.92e+13	2.92e+09	1.80e+10	6.79e+12	4.46e+11
260.00	5.49e+10	6.95e+04	1.26e+13	2.67e+09	1.71e+10	4.28e+12	3.86e+11
270.00	4.74e+10	9.68e+04	8.61e+12	2.45e+09	1.65e+10	2.80e+12	3.39e+11
280.00	4.15e+10	1.32e+05	6.04e+12	2.29e+09	1.60e+10	1.90e+12	3.01e+11
290.00	3.67e+10	1.76e+05	4.36e+12	2.14e+09	1.57e+10	1.33e+12	2.70e+11
298.00	3.36e+10	2.19e+05	3.41e+12	2.04e+09	1.55e+10	1.02e+12	2.50e+11
300.00	3.29e+10	2.31e+05	3.22e+12	2.01e+09	1.54e+10	9.55e+11	2.45e+11
310.00	2.97e+10	2.98e+05	2.43e+12	1.91e+09	1.53e+10	7.04e+11	2.25e+11
320.00	2.71e+10	3.79e+05	1.87e+12	1.81e+09	1.52e+10	5.32e+11	2.08e+11

OH + NH₂SSH

T	Γreact1	Γreact2	Γreact3
220.00	0.00	0.87	0.13
230.00	0.00	0.87	0.13
240.00	0.00	0.87	0.13
250.00	0.00	0.86	0.13
260.00	0.00	0.85	0.14
270.00	0.00	0.86	0.13

280.00	0.01	0.85	0.14
290.00	0.01	0.84	0.15
298.00	0.01	0.83	0.16
300.00	0.01	0.83	0.16
310.00	0.01	0.82	0.18
320.00	0.01	0.80	0.19

OH + NH₂SSH

T	Kbsacks react1	K fronrts react1	Kbacks react 2	K fronts react2	K pcet react3	K hat react3
220.00	9.03e+09	9.71e+05	6.23e+12	1.26e+09	6.35e+11	2.64e+11
230.00	8.03e+09	1.34e+06	4.07e+12	1.15e+09	3.66e+11	2.20e+11
240.00	7.24e+09	1.79e+06	2.77e+12	1.07e+09	2.23e+11	1.86e+11
250.00	6.60e+09	2.37e+06	1.95e+12	1.00e+09	1.43e+11	1.61e+11
260.00	6.07e+09	3.06e+06	1.42e+12	9.41e+08	9.55e+10	1.41e+11
270.00	5.65e+09	3.88e+06	1.06e+12	8.95e+08	6.65e+10	9.90e+10
280.00	5.29e+09	4.85e+06	8.11e+11	8.54e+08	4.80e+10	8.84e+10
290.00	4.99e+09	5.99e+06	6.33e+11	8.18e+08	3.56e+10	7.99e+10
298.00	4.79e+09	7.02e+06	5.26e+11	7.94e+08	2.86e+10	7.40e+10
300.00	4.74e+09	7.30e+06	5.06e+11	7.89e+08	2.71e+10	7.27e+10
310.00	4.52e+09	8.80e+06	4.09e+11	7.65e+08	2.12e+10	6.69e+10

320.00	4.34e+09	1.05e+07	3.37e+11	7.44e+08	1.70e+10	6.19e+10
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OH + (COOH)SSH

T	Гreact1	Гreact 2	Гreact3	Гreact 12
220.00	0.00	0.00	1.00	0.00
230.00	0.00	0.00	1.00	0.00
240.00	0.00	0.00	1.00	0.00
250.00	0.00	0.00	1.00	0.00
260.00	0.00	0.00	1.00	0.00
270.00	0.00	0.00	1.00	0.00
280.00	0.00	0.00	0.99	0.00
290.00	0.01	0.00	0.99	0.00
298.00	0.01	0.00	0.99	0.00
300.00	0.01	0.00	0.99	0.00
310.00	0.01	0.00	0.99	0.00
320.00	0.01	0.00	0.99	0.00

OH + (COOH)SSH

T	k backs react1	K fronts react1	K backs react2	K fronts react2	K react3	K pcet react 12
220.00	2.51e+09	2.58e+03	1.77e+06	5.53e+02	4.37e+12	3.91e+09
230.00	2.30e+09	4.00e+03	2.12e+06	9.11e+02	2.68e+12	2.67e+09
240.00	2.14e+09	6.01e+03	2.51e+06	1.45e+03	1.72e+12	1.92e+09
250.00	2.00e+09	8.75e+03	2.93e+06	2.23e+03	1.15e+12	1.43e+09
260.00	1.89e+09	1.24e+04	3.40e+06	3.33e+03	7.98e+11	1.10e+09
270.00	1.79e+09	1.71e+04	3.89e+06	4.82e+03	5.70e+11	8.78e+08
280.00	1.71e+09	2.31e+04	4.45e+06	6.81e+03	4.20e+11	7.18e+08
290.00	1.65e+09	3.06e+04	5.03e+06	9.43e+03	3.11e+11	5.99e+08
298.00	1.60e+09	3.80e+04	5.52e+06	1.20e+04	2.51e+11	5.27e+08
300.00	1.59e+09	4.00e+04	5.65e+06	1.28e+04	2.38e+11	5.10e+08
310.00	1.54e+09	5.11e+04	6.32e+06	1.70e+04	1.87e+11	4.43e+08
320.00	1.51e+09	6.47e+04	6.99e+06	2.23e+04	1.49e+11	3.91e+08

OH + CNSSH

T	$\Gamma_{\text{reaction1}}$	$\Gamma_{\text{reaction2}}$	$\Gamma_{\text{reaction3}}$
220.00	0.05	0.00	0.95
230.00	0.06	0.00	0.94
240.00	0.06	0.00	0.94

250.00	0.06	0.00	0.93
260.00	0.07	0.00	0.93
270.00	0.07	0.00	0.92
280.00	0.08	0.00	0.92
290.00	0.08	0.00	0.91
298.00	0.09	0.00	0.91
300.00	0.09	0.00	0.91
310.00	0.09	0.00	0.91
320.00	0.09	0.00	0.90

OH + CNSSH

T	K backs react1	k backs react2	k react3
220.00	6.63e+09	1.22e+08	1.25e+11
230.00	5.86e+09	1.22e+08	9.97e+10
240.00	5.23e+09	1.22e+08	8.16e+10
250.00	4.74e+09	1.22e+08	6.81e+10
260.00	4.32e+09	1.23e+08	5.79e+10
270.00	3.98e+09	1.25e+08	4.99e+10
280.00	3.70e+09	1.26e+08	4.36e+10

290.00	3.46e+09	1.28e+08	3.85e+10
298.00	3.29e+09	1.30e+08	3.52e+10
300.00	3.26e+09	1.30e+08	3.45e+10
310.00	3.08e+09	1.33e+08	3.11e+10
320.00	2.93e+09	1.35e+08	2.83e+10

OH + NO₂SSH

T	Γreaction1	Γreaction2	Γreaction3	Γreaction8
220.00	0.01	0.00	0.99	0.00
230.00	0.01	0.00	0.98	0.00
240.00	0.02	0.00	0.98	0.00
250.00	0.02	0.00	0.98	0.00
260.00	0.02	0.00	0.97	0.00
270.00	0.03	0.00	0.97	0.00
280.00	0.04	0.00	0.96	0.00
290.00	0.04	0.00	0.95	0.00
298.00	0.05	0.00	0.95	0.00
300.00	0.05	0.00	0.95	0.00

310.00	0.05	0.00	0.94	0.01
320.00	0.06	0.00	0.93	0.01

OH + NO₂SSH

T	Kbacks react1	K fronts react1	K backs react2	K fronts react2	K react3
220.00	4.67e+09	4.85e+02	2.48e+07	1.40e+08	3.98e+11
230.00	4.15e+09	8.43e+02	2.81e+07	1.49e+08	2.82e+11
240.00	3.73e+09	1.39e+03	3.17e+07	1.58e+08	2.07e+11
250.00	3.38e+09	2.23e+03	3.54e+07	1.67e+08	1.57e+11
260.00	3.11e+09	3.44e+03	3.95e+07	1.77e+08	1.22e+11
270.00	2.88e+09	5.15e+03	4.39e+07	1.86e+08	8.59e+10
280.00	2.69e+09	7.47e+03	4.84e+07	1.97e+08	6.91e+10
290.00	2.53e+09	1.06e+04	5.33e+07	2.06e+08	5.66e+10
298.00	2.42e+09	1.39e+04	5.73e+07	2.15e+08	4.89e+10
300.00	2.40e+09	1.48e+04	5.83e+07	2.16e+08	4.72e+10
310.00	2.28e+09	2.02e+04	6.38e+07	2.28e+08	4.01e+10
320.00	2.19e+09	2.70e+04	6.93e+07	2.38e+08	3.45e+10

Table S3: Main topological parameters (density ρ and laplacian of the density $\nabla^2\rho$, in a.u.) of selected transition states in the attack of the OH radical to the S atoms of the HSSR compounds.

Reaction	Property	Attack to S1				Attack to S2			
		backside		frontside		backside		frontside	
		OS	SS	OS	SS	OS	SS	OS	SS
HSSH + OH	ρ	0.0739	0.1402	0.1516	0.1265				
	$\nabla^2\rho$	0.1627	-0.1030	-0.0575	-0.0699				
HSSCH₃ + OH	ρ	0.0787	0.1443	0.1575	0.1273	0.0743	0.1438	0.1493	0.1266
	$\nabla^2\rho$	0.1604	-0.1138	-0.0978	-0.0710	0.1610	-0.1142	-0.0481	-0.0706
HSSNH₂ + OH	ρ	0.0900	0.1321	0.1538	0.1171	0.0819	0.1395	0.1698	0.1257
	$\nabla^2\rho$	0.1505	-0.0780	-0.0790	-0.0447	0.1611	-0.1002	-0.1764	-0.0651
HSSCOOH + OH	ρ	0.0788	0.1411	0.1408	0.1295	0.0869	0.1372	0.1595	0.1368
	$\nabla^2\rho$	0.1633	-0.1110	0.0041	-0.0853	0.1590	-0.1009	-0.0853	-0.1046
HSSCN + OH	ρ	0.0683	0.1375	0.1332	0.1279	0.0929	0.1335	0.1535	0.1344
	$\nabla^2\rho$	0.1608	-0.0981	0.0395	-0.0811	0.1606	-0.0819	-0.0375	-0.0976
HSSNO₂ + OH	ρ	0.0940	0.1462	0.1441	0.1331	0.1075	0.1454	0.1410	0.1675
	$\nabla^2\rho$	0.1546	-0.1092	-0.0152	-0.0864	0.1483	-0.1016	0.0332	-0.1832

a) Computed at BH&HLYP optimized geometries

Table S4: Calculated rate constants (in $M^{-1}\cdot s^{-1}$) for reactions 4, to 8 and the corresponding branching ratios (Γ in %).

Reactions 4, 5, and 6 for R = H

T	k-tot	K-R4	k-R5	k-R6	Γ -R4	Γ -R5	Γ -R6
220.00	2.85e+08	2.58e+03	3.69e+06	2.81e+08	0.00	1.29	98.70
230.00	3.02e+08	4.18e+03	3.82e+06	2.99e+08	0.00	1.26	98.74
240.00	3.21e+08	6.55e+03	4.02e+06	3.17e+08	0.00	1.25	98.75
250.00	3.40e+08	9.93e+03	4.29e+06	3.36e+08	0.00	1.26	98.74
260.00	3.61e+08	1.46e+04	4.64e+06	3.57e+08	0.00	1.28	98.71
270.00	3.84e+08	2.11e+04	5.04e+06	3.78e+08	0.01	1.31	98.68
280.00	4.06e+08	2.95e+04	5.52e+06	4.01e+08	0.01	1.36	98.64
290.00	4.30e+08	4.07e+04	6.04e+06	4.24e+08	0.01	1.40	98.59
298.00	4.50e+08	5.18e+04	6.54e+06	4.43e+08	0.01	1.45	98.53
300.00	4.55e+08	5.50e+04	6.68e+06	4.48e+08	0.01	1.47	98.52
310.00	4.81e+08	7.32e+04	7.35e+06	4.74e+08	0.02	1.53	98.46
320.00	5.09e+08	9.59e+04	8.11e+06	5.01e+08	0.02	1.59	98.39

Reactions 4, 5, and 6 for R = CH₃

T	k-tot	K-R4	k-R5	k-R6	Γ -R4	Γ -R5	Γ -R6
220.00	3.83e+09	7.86e+03	2.48e+09	1.35e+09	0.00	64.73	35.27
230.00	3.04e+09	1.14e+04	1.76e+09	1.28e+09	0.00	57.81	42.19
240.00	2.54e+09	1.61e+04	1.31e+09	1.23e+09	0.00	51.41	48.59
250.00	2.21e+09	2.24e+04	1.01e+09	1.20e+09	0.00	45.62	54.38
260.00	1.98e+09	3.03e+04	8.01e+08	1.18e+09	0.00	40.53	59.47
270.00	1.82e+09	4.05e+04	6.57e+08	1.16e+09	0.00	36.15	63.85
280.00	1.70e+09	5.32e+04	5.52e+08	1.15e+09	0.00	32.43	67.57
290.00	1.63e+09	6.89e+04	4.76e+08	1.15e+09	0.00	29.21	70.78
298.00	1.58e+09	8.37e+04	4.28e+08	1.16e+09	0.01	27.04	72.96
300.00	1.58e+09	8.78e+04	4.18e+08	1.16e+09	0.01	26.53	73.46
310.00	1.55e+09	1.11e+05	3.74e+08	1.17e+09	0.01	24.20	75.79
320.00	1.52e+09	1.38e+05	3.40e+08		0.01	22.35	77.64

				1.18e+09			
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Reactions 7 and 8 for R = CH₃

T	k-total	K-R7	k-R8	Γ-R7	Γ-R8
220.00	2.05e+08	5.79e+05	2.05e+08	0.28	99.72
230.00	1.92e+08	7.66e+05	1.91e+08	0.40	99.60
240.00	1.83e+08	9.92e+05	1.82e+08	0.54	99.46
250.00	1.78e+08	1.27e+06	1.77e+08	0.71	99.29
260.00	1.75e+08	1.59e+06	1.74e+08	0.91	99.09
270.00	1.74e+08	1.98e+06	1.72e+08	1.14	98.86
280.00	1.74e+08	2.42e+06	1.72e+08	1.39	98.61
290.00	1.75e+08	2.94e+06	1.72e+08	1.68	98.32
298.00	1.78e+08	3.41e+06	1.74e+08	1.91	98.09
300.00	1.78e+08	3.54e+06	1.75e+08	1.99	98.01
310.00	1.82e+08	4.20e+06	1.77e+08	2.31	97.69
320.00	1.86e+08	4.97e+06	1.81e+08	2.67	97.33

Reactions 4, 5, and 6 for R = NH₂

# T	k-tot	K-R4	k-R5	k-R6	Γ-R4	Γ-R5	Γ-R6
220.00	8.49e-01	1.28e-07	4.94e-01	3.55e-01	0.00	58.14	41.86
230.00	1.55e+00	5.13e-07	7.92e-01	7.63e-01	0.00	50.96	49.04
240.00	2.79e+00	1.83e-06	1.24e+00	1.55e+00	0.00	44.54	55.46
250.00	4.91e+00	5.99e-06	1.91e+00	3.00e+00	0.00	38.97	61.03
260.00	8.44e+00	1.79e-05	2.89e+00	5.55e+00	0.00	34.24	65.76
270.00	1.42e+01	4.96e-05	4.30e+00	9.86e+00	0.00	30.36	69.64
280.00	2.33e+01	1.28e-04	6.28e+00	1.70e+01	0.00	27.00	73.00
290.00	3.73e+01	3.12e-04	9.04e+00	2.83e+01	0.00	24.21	75.79
298.00	5.37e+01	6.10e-04	1.20e+01	4.17e+01	0.00	22.35	77.65
300.00	5.86e+01	7.18e-04	1.29e+01	4.58e+01	0.00	21.92	78.08
310.00	9.02e+01	1.57e-03	1.81e+01	7.21e+01	0.00	20.02	79.98
320.00	1.36e+02	3.30e-03	2.49e+01	1.11e+02	0.00	18.37	81.63

Reactions 7 and 8 for R = NH₂

T	k-total	K-R7	k-R8	Γ-R7	Γ-R8
220.00	1.24e+07	1.97e-01	1.24e+07	0.00	100.00
230.00	1.34e+07	4.83e-01	1.34e+07	0.00	100.00
240.00	1.46e+07	1.11e+00	1.46e+07	0.00	100.00
250.00	1.60e+07	2.38e+00	1.60e+07	0.00	100.00
260.00	1.76e+07	4.84e+00	1.76e+07	0.00	100.00
270.00	1.94e+07	9.42e+00	1.94e+07	0.00	100.00
280.00	2.13e+07	1.75e+01	2.13e+07	0.00	100.00
290.00	2.33e+07	3.12e+01	2.33e+07	0.00	100.00
298.00	2.51e+07	4.85e+01	2.51e+07	0.00	100.00
300.00	2.56e+07	5.38e+01	2.56e+07	0.00	100.00
310.00	2.81e+07	8.99e+01	2.81e+07	0.00	100.00
320.00	3.07e+07	1.46e+02	3.07e+07	0.00	100.00

Reactions 4, 5, and 6 for R = COOH

T	k-tot	K-R4	k-R5	k-R6	Γ-R4	Γ-R5	Γ-R6
220.00	2.59e+10	1.37e+02	1.42e+05	2.59e+10	0.00	0.00	100.00
230.00	1.53e+10	2.24e+02	1.61e+05	1.53e+10	0.00	0.00	100.00
240.00	9.54e+09	3.54e+02	1.81e+05	9.54e+09	0.00	0.00	100.00
250.00	6.27e+09	5.43e+02	2.03e+05	6.27e+09	0.00	0.00	100.00
260.00	4.30e+09	8.10e+02	2.28e+05	4.30e+09	0.00	0.01	99.99
270.00	3.07e+09	1.18e+03	2.53e+05	3.07e+09	0.00	0.01	99.99
280.00	2.27e+09	1.68e+03	2.82e+05	2.27e+09	0.00	0.01	99.99
290.00	1.73e+09	2.35e+03	3.14e+05	1.73e+09	0.00	0.02	99.98
298.00	1.42e+09	3.03e+03	3.39e+05	1.42e+09	0.00	0.02	99.98
300.00	1.36e+09	3.22e+03	3.47e+05	1.35e+09	0.00	0.03	99.97
310.00	1.09e+09	4.35e+03	3.83e+05	1.09e+09	0.00	0.04	99.96
320.00	8.95e+08	5.80e+03	4.20e+05	8.94e+08	0.00	0.05	99.95

Reactions 7 and 8 for R = COOH

T	k-total	K-R7	k-R8	Γ -R7	Γ -R8
220.00	1.87e+07	6.53e-05	1.87e+07	0.00	100.00
230.00	1.66e+07	2.23e-04	1.66e+07	0.00	100.00
240.00	1.51e+07	6.91e-04	1.51e+07	0.00	100.00
250.00	1.40e+07	1.96e-03	1.40e+07	0.00	100.00
260.00	1.32e+07	5.16e-03	1.32e+07	0.00	100.00
270.00	1.27e+07	1.27e-02	1.27e+07	0.00	100.00
280.00	1.22e+07	2.93e-02	1.22e+07	0.00	100.00
290.00	1.20e+07	6.41e-02	1.20e+07	0.00	100.00
298.00	1.19e+07	1.16e-01	1.19e+07	0.00	100.00
300.00	1.19e+07	1.33e-01	1.19e+07	0.00	100.00
310.00	1.18e+07	2.66e-01	1.18e+07	0.00	100.00
320.00	1.18e+07	5.08e-01	1.18e+07	0.00	100.00

Reactions 4, 5, and 6 for R = CN

T	k-tot	K-R4	k-R5	k-R6	Γ -R4	Γ -R5	Γ -R6
220.00	7.42e+09	3.50e-03	7.30e+09	1.16e+08	0.00	98.43	1.57
230.00	5.91e+09	1.04e-02	5.81e+09	1.07e+08	0.00	98.19	1.81
240.00	4.83e+09	2.81e-02	4.73e+09	1.01e+08	0.00	97.91	2.09
250.00	4.03e+09	7.06e-02	3.94e+09	9.65e+07	0.00	97.61	2.39
260.00	3.42e+09	1.66e-01	3.33e+09	9.36e+07	0.00	97.27	2.73
270.00	2.95e+09	3.69e-01	2.86e+09	9.18e+07	0.00	96.89	3.11
280.00	2.59e+09	7.76e-01	2.50e+09	9.11e+07	0.00	96.48	3.52
290.00	2.30e+09	1.56e+00	2.21e+09	9.09e+07	0.00	96.05	3.95
298.00	2.11e+09	2.64e+00	2.01e+09	9.11e+07	0.00	95.67	4.33
300.00	2.06e+09	3.01e+00	1.97e+09	9.13e+07	0.00	95.57	4.43
310.00	1.87e+09	5.57e+00	1.78e+09	9.23e+07	0.00	95.06	4.94
320.00	1.71e+09	9.94e+00	1.62e+09	9.37e+07	0.00	94.53	5.47

Reactions 7 and 8 for R = CN

T	k-total	K-R7	k-R8	Γ -R7	Γ_n -R8
220.00	2.78e+07	3.95e-01	2.78e+07	0.00	100.00
230.00	2.42e+07	9.24e-01	2.42e+07	0.00	100.00
240.00	2.16e+07	2.02e+00	2.16e+07	0.00	100.00
250.00	1.98e+07	4.17e+00	1.98e+07	0.00	100.00
260.00	1.84e+07	8.17e+00	1.84e+07	0.00	100.00
270.00	1.75e+07	1.53e+01	1.75e+07	0.00	100.00
280.00	1.67e+07	2.75e+01	1.67e+07	0.00	100.00
290.00	1.62e+07	4.76e+01	1.62e+07	0.00	100.00
298.00	1.60e+07	7.21e+01	1.60e+07	0.00	100.00
300.00	1.59e+07	7.97e+01	1.59e+07	0.00	100.00
310.00	1.57e+07	1.29e+02	1.57e+07	0.00	100.00
320.00	1.56e+07	2.05e+02	1.56e+07	0.00	100.00

Reactions 4, 5, and 6 for R = NO₂

T	k-tot	K-R4	k-R5	k-R6	Γ -R4	Γ -R5	Γ -R6
220.00	1.64e+08	2.19e+05	1.63e+08	1.14e+06	0.13	99.17	0.69
230.00	1.20e+08	2.50e+05	1.18e+08	1.23e+06	0.21	98.76	1.03
240.00	9.05e+07	2.85e+05	8.89e+07	1.34e+06	0.32	98.20	1.48
250.00	7.10e+07	3.23e+05	6.92e+07	1.47e+06	0.45	97.48	2.07
260.00	5.71e+07	3.65e+05	5.52e+07	1.60e+06	0.64	96.56	2.81
270.00	4.72e+07	4.10e+05	4.51e+07	1.76e+06	0.87	95.41	3.72
280.00	4.01e+07	4.58e+05	3.77e+07	1.92e+06	1.14	94.07	4.79
290.00	3.48e+07	5.13e+05	3.22e+07	2.10e+06	1.47	92.49	6.04
298.00	3.15e+07	5.59e+05	2.87e+07	2.25e+06	1.77	91.07	7.16
300.00	3.08e+07	5.70e+05	2.79e+07	2.29e+06	1.85	90.69	7.45
310.00	2.77e+07	6.33e+05	2.46e+07	2.51e+06	2.29	88.67	9.04
320.00	2.54e+07	7.01e+05	2.20e+07	2.74e+06	2.76	86.46	10.78

Reactions 7 and 8 for R = NO₂

T	k-total	K-R7	k-R8	Г-R7	Г-R8
220.00	8.96e+09	6.99e-04	8.96e+09	0.00	100.00
230.00	6.24e+09	2.21e-03	6.24e+09	0.00	100.00
240.00	4.54e+09	6.37e-03	4.54e+09	0.00	100.00
250.00	3.44e+09	1.70e-02	3.44e+09	0.00	100.00
260.00	2.68e+09	4.21e-02	2.68e+09	0.00	100.00
270.00	2.16e+09	9.79e-02	2.16e+09	0.00	100.00
280.00	1.77e+09	2.16e-01	1.77e+09	0.00	100.00
290.00	1.49e+09	4.53e-01	1.49e+09	0.00	100.00
298.00	1.32e+09	7.91e-01	1.32e+09	0.00	100.00
300.00	1.28e+09	9.05e-01	1.28e+09	0.00	100.00
310.00	1.12e+09	1.74e+00	1.12e+09	0.00	100.00
320.00	9.84e+08	3.21e+00	9.84e+08	0.00	100.00

Table S5: Absolute energies and enthalpic and entropic corrections (in hartree), Zero point energies (ZPVE in kcal·mol⁻¹) and entropy (S in cal·mol⁻¹·K⁻¹).

OH + HSSH

	Energy	ZPVE	H correction	G correction	S	Energy	Energy
	BH&HLYP	BH&HLYP	BH&HLYP	BH&HLYP	BH&HLYP	CCSD(T)//BH&HLYP	CCSD(T)//QCISD
OH	-75.73240	5.6	0.01216	-0.00804	52.5	-75.645461	-75.645568
HSO	-473.96206	6.8	0.01467	-0.01270	57.5	-473.423482	
HOS	-473.96204	8.7	0.01768	-0.00951	57.2	-473.421538	
HSSH	-797.60461	11.9	0.02331	-0.00588	61.6	-796.687438	-796.687565
HSOH	-474.58680	14.8	0.02763	0.00005	58.1	-474.051572	-474.052049
SH	-398.75697	3.9	0.00959	-0.01221	45.9	-398.293266	-398.293305
HSO	-473.96206	6.8	0.01467	-0.01270	57.5	-473.423482	
SH2	-399.40130	9.8	0.01934	-0.00463	50.5	-398.943541	
HS2	-796.98591	6.1	0.01364	-0.01522	60.7	-796.063886	-796.063886
H2O	-76.41851	13.9	0.02599	0.00461	45.0	-76.342005	-76.342285
Reaction 1							
HSSH + OH	-873.33700	17.5	0.03546	-0.01392	114.1	-872.332899	-872.333133
CRFTS1a	-873.34206	19.0	0.03750	-0.00038	79.7	-872.339808	-872.340316
FTS1a	-873.31599	19.8	0.03753	0.00309	72.5	-872.326442	-872.326940
CPFTS1a	-873.34717	19.7	0.03889	-0.00049	82.9	-872.349684	-872.350374
CRFTS1b	-873.34054	18.8	0.03740	-0.00208	83.1	-872.337962	-872.338255
FTS1b	-873.31967	20.2	0.03798	0.00370	72.2	-872.330018	-872.330437
CPFTS1b	-873.34733	20.0	0.03903	0.00084	80.4	-872.350089	-872.350380
CRBTS1a	-873.34053	18.5	0.03725	-0.00340	85.5	-872.337307	-872.338255

BTS1a	-873.33692	19.5	0.03735	0.00214	74.1	-872.340147	-872.338830
CPBTS1a	-873.34708	20.7	0.03951	0.00412	74.5	-872.354013	-872.354767
CRBTS1b	-873.34205	19.0	0.03750	-0.00043	79.8	-872.339812	-872.340319
BTS1b	-873.33866	19.6	0.03741	0.00235	73.8	-872.341303	-872.339399
CPBTS1b	-873.34642	20.5	0.03931	0.00359	75.2	-872.352896	-872.353637
Reaction 3							
CRPTS3a	-873.34205	19.0	0.03748	-0.00046	79.8	-872.339836	-872.340319
PTS3a	-873.32227	18.0	0.03450	-0.00036	73.4	-872.329456	-872.329895
CPPTS3a	-873.41149	21.8	0.04201	0.00367	80.7	-872.414634	-872.415010
CRHTS3a	-873.34053	18.6	0.03727	-0.00336	85.5	-872.337307	-872.338255
HTS3a	-873.33673	17.5	0.03434	-0.00233	77.2	-872.335688	-872.335749
CPHTS3a	-873.41148	21.8	0.04201	0.00364	80.7	-872.414634	-872.415010
CRHTS3b	-873.34205	19.0	0.03750	-0.00043	79.8	-872.339836	-872.340319
HTS3b	-873.33623	17.4	0.03430	-0.00245	77.3	-872.335293	-872.335329
CPHTS3b	-873.40802	21.3	0.04181	0.00032	87.3	-872.411005	-872.411525
HSOH·SH	-873.35243	20.6	0.03932	0.00306	76.3	-872.355717	
TSTRF	-873.32826	15.7	0.03132	-0.00508	76.6	-872.332287	
Reaction 5							
HSOH + SH	-873.34377	18.6931	0.03722	-0.01216	103.9	-872.344839	
CRHTS5a	-873.35243	20.6	0.03932	0.00306	76.3	-872.355717	
HTS5a	-873.32826	15.7	0.03132	-0.00508	76.6	-872.332287	
CPHTS5a	-873.36764	17.9	0.03617	-0.00365	83.8	-872.373374	
CRHTS5b	-873.35132	20.4	0.03915	0.00252	77.1	-872.354630	
HTS5b	-873.32823	15.6	0.03125	-0.00520	76.7	-872.332128	
CPHTS5b	-873.36764	17.8	0.03616	-0.00370	83.9	-872.373377	
HSO + SH₂	-873.36336	16.6	0.03401	-0.01733	108.0	-872.367023	
Rection 6							
CRHTS6a	-873.34732	20.0	0.03902	0.00079	80.5	-872.350083	
HTS6a	-873.33776	17.0	0.03351	-0.00302	76.9	-872.341826	

CPHTS6a	-873.37077	20.0	0.03934	-0.00026	83.3	-872.374578	
CRHTS6b	-873.35243	20.6	0.03932	0.00307	76.3	-872.355719	
HTS6b	-873.33738	17.0	0.03359	-0.00294	76.9	-872.341564	
CPTHS6b	-873.37079	20.0	0.03934	-0.00040	83.6	-872.374569	

OH + CH₃SSH

SH₂	-399.40130	9.8	0.01934	-0.00463	50.5	-398.94354	
CH₃SH	-438.69719	29.8	0.05195	0.02325	60.4	-438.18021	
CH₃SO	-513.27380	26.1	0.04655	0.01470	67.0	-512.67676	
CH₃SSH	-836.90564	31.0	0.05516	0.02179	70.2	-835.93079	-835.93112
CH₃S	-438.05870	23.1	0.04085	0.01251	59.6	-437.53542	-437.53565
CH₃SOH	-513.89135	33.8	0.05923	0.02746	66.9	-513.29756	-513.29821
CH₂SSH	-836.24643	21.6	0.04041	0.00592	72.6		
Reaction 1							
CRBTS1a	-912.64166	37.6	0.06909	0.02434	94.2	-911.58079	-911.58110
BTS1a	-912.63697	38.7	0.06941	0.02991	83.1	-911.58311	-911.58225
CPBTS1a	-912.64538	39.9	0.07170	0.03152	84.6	-911.59545	-911.59644
CRBTS1b	-912.64236	37.9	0.06933	0.02613	90.9	-911.58244	-911.58272
BTS1b	-912.63960	38.8	0.06949	0.03034	82.4	-911.58571	-911.58412
CPBTS1b	-912.64457	39.8	0.07154	0.03155	84.2	-911.59431	-911.59529
CRFTS1b	-912.64165	37.6	0.06912	0.02436	94.2	-911.58079	-911.58110
FTS1b	-912.61980	39.1	0.06976	0.03087	81.9	-911.57288	-911.57353
CPFTS1b	-912.65327	39.3	0.07130	0.02692	93.4	-911.59738	-911.59830
CRFTS1a	-912.64235	37.9	0.06934	0.02594	91.3	-911.58244	-911.58272
FTS1a	-912.61397	39.1	0.06974	0.03106	81.4	-911.56710	-911.56776
CPFTS1a	-912.64456	39.8	0.07150	0.03137	84.5	-911.59430	-911.59529
Reaction 2							
CRBTS2a	-912.64401	38.3	0.06964	0.02820	87.2	-911.58613	-911.58800
BTS2a	-912.64082	38.5	0.06910	0.03018	81.9	-911.58815	-911.58694

CPBTS2a	-912.65213	39.3	0.07095	0.03064	84.8	-911.60085	-911.60279
CRBTS2b	-912.64584	38.5	0.06971	0.02918	85.3	-911.58855	-911.59031
BTS2b	-912.64303	38.6	0.06915	0.03049	81.4	-911.58964	-911.58894
CPBTS2b	-912.65416	38.9	0.07059	0.02863	88.3	-911.59896	-911.59940
CRFTS2b	-912.64401	38.3	0.06962	0.02823	87.1	-911.58613	-911.58800
FTS2b	-912.62704	39.1	0.06969	0.03131	80.8	-911.58052	-911.58118
CPFTS2b	-912.66070	39.5	0.07094	0.03132	83.4	-911.60692	-911.60789
CRFTS2a	-912.64585	38.5	0.06972	0.02920	85.3	-911.58849	-911.59031
FTS2a	-912.62306	38.7	0.06928	0.03061	81.4	-911.57656	-911.57729
CPFTS2a	-912.65408	38.9	0.07065	0.02817	89.4	-911.59880	-911.59940
Reaction 5							
CR5a	-912.65328	39.3	0.07131	0.02713	93.0	-911.59738	
HTS5a	-912.62656	35.1	0.06359	0.02311	85.2	-911.57437	
CP5a	-912.66391	37.5	0.06876	0.02402	94.2	-911.61078	
CR5b	-912.65328	39.3	0.07131	0.02713	93.0	-911.59738	
HTS5b	-912.62613	35.0	0.06366	0.02189	87.9	-911.57224	
CP5b	-912.66391	37.5	0.06876	0.02402	94.2	-911.61078	
Reactio 6							
CR6a	-912.64947	38.8	0.07078	0.02581	94.7	-911.59373	
HTS6a	-912.63724	36.6	0.06617	0.02529	86.0	-911.58396	
CP6a	-912.66879	39.9	0.07199	0.02906	90.3	-911.61413	
CR6b	-912.65328	39.3	0.07130	0.02687	93.5	-911.59738	
HTS6b	-912.63586	36.5	0.06607	0.02382	88.9	-911.58199	
CP6b	-912.66863	39.9	0.07198	0.02885	90.8	-911.61384	
Reaction 8							
CR8a	-912.66070	39.5	0.07093	0.03129	83.4	-911.60693	
HTS8a	-912.63840	34.7	0.06310	0.02288	84.7	-911.58362	
CP8a	-912.67927	36.9	0.06801	0.02284	95.1	-911.62636	
CR8b	-912.65876	39.4	0.07080	0.03080	84.2	-911.60483	

HTS8b	-912.63845	34.6	0.06301	0.02274	84.8	-911.58349	
CP6b	-912.67916	36.8	0.06801	0.02264	95.5	-911.62636	
Reaction 11							
CRHST11a	-912.64299	37.9	0.06911	0.02645	89.8	-911.58252	-911.58296
HTS11a	-912.62768	34.9	0.06334	0.02327	84.3	-911.57364	-911.57392
CPHTS11a	-912.66775	36.7	0.06860	0.02119	99.8	-911.61348	-911.61424
CRHTS11b	-912.64333	37.8	0.06909	0.02565	91.4	-911.58251	-911.58296
HTS11b	-912.62699	34.7	0.06328	0.02233	86.2	-911.57245	-911.57247
CPHTS11b	-912.66776	36.7	0.06859	0.02116	99.8	-911.61347	-911.61424
Reaction 3							
CRPTS3a	-912.64584	38.5	0.06970	0.02915	85.4	-911.58851	-911.59031
PTS3a	-912.63000	37.4	0.06675	0.02904	79.4	-911.58147	-911.58228
CPPTS3a	-912.71560	40.8	0.07396	0.03033	91.8	-911.66163	-911.66163
CRPTS3b	-912.64584	38.5	0.06970	0.02913	85.4	-911.58850	-911.59031
PTS3b	-912.62621	36.8	0.06625	0.02752	81.5	-911.57678	-911.57796
CPPTS3b	-912.71560	40.8	0.07397	0.03035	91.8	-911.66163	-911.66163
CRHTS3a	-912.64584	38.5	0.06970	0.02913	85.4	-911.58850	-911.59031
HST3a	-912.63887	36.7	0.06655	0.02569	86.0	-911.58002	-911.58034
CPHTS3a	-912.71559	40.8	0.07397	0.03035	91.8	-911.66163	-911.66163
CRHTS3b	-912.64235	37.9	0.06934	0.02596	91.3	-911.58244	-911.58272
HTS3b	-912.63792	36.5	0.06639	0.02525	86.6		-911.57991
CPHTS3b	-912.71559	40.8	0.07397	0.03035	91.8	-911.66163	-911.66163

OH + NH₂SSH

NH₂SO	-529.31862	19.0	0.03524	0.00386	66.0	-528.71594	
NH₂SH	-454.72586	23.0	0.04087	0.01290	58.9	-454.20219	
NH₂SSH	-852.94248	24.2	0.04395	0.01146	68.4	-851.96071	-851.96123
NH₂SOH	-529.93598	27.1	0.04820	0.01733	65.0	-529.33575	-529.33654
NH₂S	-454.11109	16.4	0.03044	0.00228	59.3	-453.58077	-453.58108

<i>Reaction 1</i>							
CR1a	-928.67838	31.0	0.05801	0.01571	89.0	-927.61147	-927.61106
FTS1a	-928.65913	32.2	0.05852	0.02085	79.3	-927.60472	-927.60550
CP1b	-928.70827	32.8	0.06041	0.01917	86.8	-927.64625	-927.64713
CR1b	-928.67986	31.4	0.05816	0.01669	87.3	-927.61301	-927.61361
FTS1b	-928.65082	32.4	0.05838	0.02150	77.6	-927.59910	-927.60004
CP1c	-928.70334	32.7	0.06049	0.01765	90.2	-927.64122	-927.64227
CR1b	-928.67986	31.4	0.05817	0.01679	87.1	-927.61301	-927.61361
BTS1b	-928.67179	31.5	0.05782	0.01876	82.2	-927.61050	-927.60938
CP1a	-928.70388	32.4	0.06021	0.01789	89.1	-927.64148	-927.64220
CR1a	-928.67834	30.7	0.05786	0.01362	93.1	-927.61147	-927.61106
BTS1a	-928.67304	31.8	0.05818	0.01943	81.6	-927.61301	-927.61231
CP1a	-928.70388	32.4	0.06019	0.01780	89.2	-927.64147	-927.64220
<i>Reaction 2</i>							
CR3a	-928.68257	31.8	0.05857	0.01905	83.2	-927.61862	-927.62098
FTS2a	-928.66474	32.2	0.05823	0.02139	77.5	-927.61130	-927.61224
CP2c	-928.70463	32.7	0.05979	0.02080	82.1	-927.64434	-927.64541
CR4a	-928.68428	31.8	0.05857	0.01949	82.2	-927.62072	-927.62283
FTS2b	-928.66376	31.9	0.05808	0.02036	79.4	-927.61038	-927.61115
CP2b	-928.70027	32.4	0.05957	0.01974	83.8	-927.63919	-927.63978
CR2a	-928.68086	31.4	0.05819	0.01856	83.4	-927.61733	-927.61969
BTS2a	-928.67539	31.6	0.05782	0.01965	80.3	-927.61737	-927.61696
CP2a	-928.70027	32.4	0.05956	0.01972	83.9	-927.63920	-927.63978
CR2b	-928.67911	31.1	0.05805	0.01737	85.6	-927.61467	-927.61760
BTS2b	-928.67269	31.5	0.05771	0.01913	81.2	-927.61422	-927.61464
CP2b	-928.70027	32.4	0.05954	0.01960	84.1	-927.63919	-927.63978
<i>Reaction 3</i>							
CRHTS3b	-928.68427	31.8	0.05858	0.01950	82.2	-927.62072	-927.62283
HTS3b	-928.67536	29.8	0.05515	0.01511	84.3	-927.60980	-927.61019

CPHTS3b	-928.75414	34.0	0.06274	0.02126	87.3	-927.69411	-927.69489
CRHTS3a	-928.68026	31.1	0.05811	0.01628	88.0		-927.61423
HTS3a	-928.67430	29.6	0.05497	0.01469	84.8	-927.60902	-927.61024
CPHTS3a	-928.75413	34.0	0.06273	0.02122	87.4	-927.69411	-927.69489
CRPTS3a	-928.68087	31.4	0.05821	0.01860	83.4		-927.61969
PTS3a	-928.66356	30.3	0.05531	0.01815	78.2	-927.60929	-927.61027
CPPTS3a	-928.75119	33.9	0.06249	0.02093	87.5		-927.69276
NH2SS	-852.32669	18.3	0.03429	0.00149	69.0		
Reaction 5							
CRHTS5a	-928.70827	32.8	0.06042	0.01918	86.8	-927.64625	
HTS5a	-928.66876	29.0	0.05327	0.01496	80.6	-927.61201	
CPHTS5a	-928.69330	31.1	0.05792	0.01518	89.9	-927.63388	
CRHTS5b	-928.70722	32.6	0.06040	0.01778	90.7	-927.64425	
HTS5b	-928.66363	28.2	0.05266	0.01205	85.5	-927.60272	
CPHTS5b	-928.69330	31.1	0.05792	0.01518	89.9	-927.63388	
Reaction 6							
CRHTS6a	-928.70567	32.6	0.06040	0.01795	89.4	-927.64310	
HTS6a	-928.67497	29.9	0.05521	0.01576	83.0	-927.61510	
CPHTS6a	-928.70152	33.7	0.06141	0.02072	85.6	-927.64123	
CRHTS6b	-928.70566	32.6	0.06040	0.01792	89.4	-927.64309	
HTS6b	-928.67683	30.1	0.05535	0.01572	83.4	-927.61665	
CPHTS6b	-928.69615	32.9	0.06071	0.01639	73.6	-927.63382	
Reaction 8							
CRHTS8a	-928.70463	32.7	0.05979	0.02087	81.9	-927.64433	
HTS8a	-928.68223	27.9	0.05188	0.01262	82.6	-927.62125	
CPHTS8a	-928.72495	30.0	0.05676	0.01334	91.4	-927.66696	
CRHTS8b	-928.70463	32.7	0.05979	0.02087	81.9	-927.64433	
HTS8b	-928.68220	27.8	0.05179	0.01230	83.1	-927.62110	
CPHTS8b	-928.72472	30.0	0.05675	0.01325	91.6	-927.66675	

OH + (COOH)SSH

(COOH)SO	-662.50634	18.1	0.03490	-0.00064	74.8	-661.7514268	
(COOH)SH	-587.94572	22.1	0.04031	0.00807	67.9	-587.270045	
(COOH)SSH	-986.14972	23.0	0.04339	0.00639	77.9	-985.0168634	-985.0182332
(COOH)SOH	-663.13832	25.8	0.04752	0.01203	74.7	-662.3856897	-662.3873817
(COOH)S	-587.30407	15.9	0.03023	-0.00210	68.2	-586.622508	-586.6237621
Reaction 1							
CRBTS1a	-1061.88364	29.5	0.05733	0.00862	102.5	-1060.664461	-1060.66638
BTS1a	-1061.87921	30.7	0.05766	0.01457	990.7	-1060.667236	-1060.667198
CPBTS1a	-1061.89316	31.4	0.05986	0.01166	101.5	-1060.678555	-1060.679194
CRBTS1b	-1061.88536	29.5	0.05732	0.00855	102.7	-1060.666519	-1060.668543
BTS1b	-1061.88064	30.6	0.05755	0.01430	91.0	-1060.668353	-1060.668834
CPBTS1b	-1061.90769	32.4				-1060.69372	-1060.695211
CRFTS1a	-1061.89187	30.1	0.05758	0.01171	96.5	-1060.673245	-1060.674605
FTS1a	-1061.85758	31.4	0.05812	0.01696	86.6	-1060.653377	-1060.654894
CPFTS1b	-1061.90770	32.4	0.06024	0.01721	90.5	-1060.693724	-1060.695213
CRGTS1b	-1061.88541	29.6	0.05739	0.01006	99.6	-1060.667157	-1060.668543
FTS1b	-1061.86456	31.0	0.05786	0.01566	88.8	-1060.659388	-1060.660932
CPFTS1b	-1061.89896	32.0	0.06008	0.01597	92.8	-1060.685172	-1060.686817
Reaction 2							
CRBTS2a	-1061.88469	29.6	0.05731	0.01040	98.7	-1060.667212	-1060.668874
BTS2a	-1061.87322	30.4	0.05726	0.01456	89.9	-1060.664532	-1060.664125
CPBTS2a	-1061.89659	30.7	0.05881	0.01061	101.4	-1060.681861	-1060.683796
CRFTS2a	-1061.88626	29.7	0.05738	0.01132	96.9	-1060.66887	-1060.670742
FTS2a	-1061.85914	30.6	0.05733	0.01548	88.1	-1060.655638	-1060.657344
CPFTS2a	-1061.90330	30.9	0.05878	0.01373	94.8	-1060.689735	-1060.691579
CRFTS2b	-1061.88470	29.6	0.05732	0.01045	98.6	-1060.667218	-1060.668874
FTS2b	-1061.86144	30.8	0.05763	0.01582	88.0	-1060.657731	-1060.659358

CPFTS2b	-1061.89662	30.3	0.05862	0.00994	102.5	-1060.682586	-1060.683796
Reaction 12							
CRPTS12a	-1061.89575	30.4	0.05761	0.01383	92.1	-1060.676691	-1060.678075
PTS12a	-1061.87018	28.5	0.05356	0.01243	86.6	-1060.659519	-1060.66114
CPPTS12a	-1061.89310	29.6	0.05786	0.00791	105.1	-1060.677249	-1060.679547
CRPTS12b	-1061.89575	30.4	0.05761	0.01382	92.2	-1060.676691	-1060.678075
PTS12b	-1061.86991	28.5	0.05355	0.01242	86.6	-1060.6593	-1060.660918
CPPTS12b	-1061.89309	29.6	0.05786	0.00791	105.1	-1060.677244	-1060.679547
Reaction 3							
CRHTS3b	-1061.89187	30.1	0.05760	0.01187	96.3	-1060.673245	-1060.674605
HTS3b	-1061.88427	29.7	0.05422	0.01225	88.3	-1060.670471	-1060.671474
CPHTS3b	-1061.95281	35.6	0.06223	0.01326	103.1	-1060.739872	-1060.741598
CRHTS3a	-1061.89188	30.1	0.05760	0.01187	96.3	-1060.673245	-1060.674605
HTS3a	-1061.88085	28.2	0.05411	0.00983	93.2	-1060.664936	-1060.666146
CPHTS3b	-1061.95281	35.6	0.06223	0.01326	103.1	-1060.739872	-1060.741598
(COOH)SS	-985.52801	17.3	0.03387	-0.00301	77.6		
Reaction 5							
CRHTS5a	-1061.89561	31.5	0.05992	0.01271	99.4	-1060.681243	
HTS5a	-1061.87947	27.6	0.05251		89.9	-1060.667834	
CPHTS5a	-1061.91725	30.1	0.05734	0.01186	95.7	-1060.705339	
Reaction 6							
CRHTS6a	-1061.89974	32.1	0.06020	0.01610	92.8	-1060.686784	
HTS6a	-1061.88333	28.6	0.05443	0.01057	92.3	-1060.671885	
CPHTS6a	-1061.91233	31.6	0.06002	0.01326	98.4	-1060.698465	
Reaction 8							
CRHTS8a	-1061.90330	30.9	0.05877	0.01374	94.8	-1060.689734	
HTS8a	-1061.87470	26.6	0.05114	0.00762	91.6	-1060.663794	
CPHTS8a	-1061.91156	28.8	0.05636	0.00677	104.4	-1060.70047	
CRHTS8b	-1061.90330	30.9	0.05877	0.01374	94.8	-1060.689734	

HTS8b	-1061.87535	26.6	0.05112	0.00776	91.3	-1060.664699	
CPHTS8b	-1061.91156	28.8	0.05636	0.00677	104.4	-1060.70047	

OH + CNSSH

CHSH	-491.60527	11.0	0.02210	-0.00711	61.5	-491.02551	
CNSSH	-889.80939	12.4	0.02546	-0.00866	71.8	-888.77166	-888.77337
CNS	-490.97502	5.2	0.01234	-0.01484	57.2	-490.38769	-490.38896
CNSOH	-566.79556	15.3	0.02964	-0.00288	68.4	-566.13903	-566.14107
Reaction 1							
CRFTS1a	-965.54556	19.1	0.03945	-0.00383	91.1	-964.42267	-964.42436
FTS1a	-965.52867	20.4	0.03997	0.00093	82.2	-964.41787	-964.41962
CPFTS1a	-965.56628	20.8	0.04171	-0.00254	93.1	-964.44565	-964.44671
CRFTS1b	-965.54888	19.1	0.03932	-0.00398	91.1	-964.42564	-964.42739
FTS1b	-965.51952	20.4	0.04003	0.00005	84.1	-964.40991	-964.41182
CPFTS1b	-965.56628	20.8	0.04170	-0.00257	93.2	-964.44564	-964.44671
CRBTS1b	-965.54568	18.6	0.03918	-0.00673		-964.42267	-964.42436
BTS1b	-965.54169	19.9	0.03946	-0.00082	84.8	-964.42332	-964.42380
CPBTS1b	-965.56627	20.7	0.04169	-0.00289	93.8	-964.44564	-964.44671
CRB TS1a	-965.54888	19.0	0.03928	-0.00449	92.1	-964.42564	-964.42739
BTS1a	-965.54292	19.8	0.03940	-0.00110	85.2	-964.42393	-964.42445
CPBTS1a	-965.56627	20.7	0.04170	-0.00291	93.9	-964.44564	-964.44671
Reaction 2							
CRFTS2a	-965.55065	19.5	0.03972	-0.00404	92.1	-964.42630	-964.42804
FTS2a	-965.52349	20.2	0.03967	0.00064	82.1	-964.41419	-964.41594
CPBTS2a	-965.55408	19.5	0.04065	-0.00732	101.0	-964.43537	-964.43758
CRFTS2b	-965.54887	19.1	0.03931	-0.00404	91.2	-964.42564	-964.42739
FTS2b	-965.52017	20.0	0.03942	0.00036	82.2	-964.41103	-964.41289
CPFTS2b	-965.55409	19.6	0.04066	-0.00688	100.0	-964.43543	-964.43758
CRBTS2b	-965.55066	19.6	0.03973	-0.00397	92.0	-964.42632	-964.42804

BTS2b	-965.53341	19.7	0.03919	-0.00066	83.9	-964.41954	-964.42005
CPBTS2b	-965.55568	19.8	0.04072	-0.00414	94.4	-964.43765	-964.43982
CRBTS2a	-965.55065	19.5	0.03972	-0.00401	92.0	-964.42632	-964.42804
BTS2a	-965.53704	19.8	0.03919	-0.00026	83.0	-964.42217	-964.42225
CPBTS2a	-965.55574	19.8	0.04073	-0.00410	94.3	-964.43776	-964.43982
Reaction 3							
CRHTS3b	-965.54888	19.1	0.03931	-0.00404	91.2	-964.42564	-964.42739
HTS3b	-965.54012	17.5	0.03589	-0.00549	87.1	-964.41915	-964.42067
CPHTS3b	-965.61199	21.7	0.04401	-0.00099	94.7	-964.49482	-964.49674
CRHTS3a	-965.54888	19.1	0.03931	-0.00404	91.2	-964.42564	-964.42739
HTS3a	-965.54106	17.5	0.03585	-0.00541	86.8	-964.42030	-964.42200
CPHTS3a	-965.61199						
	-965.61199	21.7	0.04401	-0.00099	94.7	-964.49482	-964.49674
	-889.18745	6.7	0.01592	-0.01802	71.4	-888.14527	-888.14693
Reaction 5							
CRHTS5a	-965.57338	21.5	0.04188	0.00176	8.4	-964.45514	
HTS5a	-965.55286	17.5	0.03497	-0.00400	82.0	-964.43959	
CPHTS5a	-965.57729	19.1	0.03897	-0.00404	90.5	-964.46167	
Reaction 6							
CRHTS6a	-965.57338	21.5	0.04188	0.00178	84.4	-964.45515	
HTS6a	-965.55057	18.1	0.03646	-0.00375	84.6	-964.43518	
CPHTS6a	-965.57922	21.1	0.04230	-0.00271	94.7	-964.46041	
Reaction 8							
CRHTS8a	-965.56043	20.2	0.04084	-0.00297	92.2	-964.44276	
HTS8a	-965.53197	15.9	0.03319	-0.00792	86.5	-964.41659	
CPHTS8a	-965.57017	17.8	0.03822	-0.01059	102.7	-964.45579	
CRHTS8b	-965.56044	20.2	0.04084	-0.00297	92.2	-964.44276	
HTS8b	-965.53233	15.9	0.03319	-0.00788	86.4	-964.41707	
CPHTS8b	-965.57017	17.8	0.03822	-0.01059	102.7	-964.45579	

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OH + NO₂SSH

NO₂SH	-603.82929	13.4	0.02589	-0.00546	66.0	-603.15949	
NO₂SO	-678.40936	9.9	0.02103	-0.01290	71.4	-677.66174	
NO₂SSH	-1002.05363	15.1	0.03042	-0.00597	76.6	-1000.92587	-1000.92789
NO₂	-205.03310	5.9	0.01322	-0.01457	58.5	-204.81465	-204.81689
NO₂S	-603.20211	7.9	0.01718	-0.01484	67.4	-602.52623	-602.52812
Reaction 1							
CRBTS1b	-1077.78978	21.3	0.04414	-0.00420	101.7	-1076.57556	-1076.57763
BTS1b	-1077.78140	22.8	0.04480	0.00252	89.0	-1076.57618	-1076.57695
CPBTS1b	-1077.79809	23.9	0.04701	0.00325	92.1	-1076.58869	-1076.59085
CRBTS1a	-1077.79303	21.8	0.04432	-0.00141	96.2	-1076.57967	-1076.58169
BTS1a	-1077.78426	22.8	0.04462	0.00259	88.5	-1076.57813	-1076.57909
CPBTS1a	-1077.80414	24.2	0.04709	0.00412	90.4	-1076.59449	-1076.59654
CRFTS1b	-1077.79304	21.7	0.04335	0.00014	90.9	-1076.57967	-1076.58169
FTS1b	-1077.75683	22.8	0.04449	0.00305	87.2	-1076.55721	-1076.55949
CPFTS1b	-1077.79808	23.9	0.04700	0.00321	92.2	-1076.58869	-1076.59085
CRFTS1a	-1077.78912	21.7	0.04432	-0.00175	97.0	-1076.57462	-1076.57519
FTS1a	-1077.76629	23.0	0.04488	0.00343	87.2	-1076.56622	-1076.56858
CPFTS1a	-1077.79808	23.9	0.04702	0.00320	92.2	-1076.58869	-1076.59085
Reaction 2							
CRBTS2a	-1077.79154	21.9	0.04439	-0.00201	97.7	-1076.57759	-1076.57781
BTS2a	-1077.77144	22.2	0.04411	0.00149	87.7	-1076.57120	-1076.57283
CPBTS2a	-1077.80310	22.7	0.04585	-0.00207	100.9	-1076.59334	-1076.59407
CRBTS2b	-1077.79064	21.6	0.04433	-0.00210	97.7	-1076.57807	-1076.57769
BTS2b	-1077.77636	22.4	0.04418	0.00202	88.7	-1076.57427	-1076.57474
CPBTS2b	-1077.80311	22.7	0.04584	-0.00224	101.2	-1076.59334	-1076.59407
Reaction 10							

CRFTS10b	-1077.78887	21.5	0.04428	-0.00356	100.7	-1076.57624	-1076.57998
FTS10b	-1077.77201	22.7	0.04459	0.00255	88.5	-1076.57321	-1076.57538
CPFTS10b	-1077.84027	22.5	0.04605	-0.00475	106.9	-1076.63094	-1076.63436
CRFTS10a	-1077.79064	21.6	0.04433	-0.00199	97.5	-1076.57806	-1076.57769
FTS10a	-1077.77230	22.5	0.04435	0.00210	88.9	-1076.57376	-1076.57593
CPFTS10a	-1077.83991	22.5	0.04608	-0.00500	107.5	-1076.62953	-1076.63321
Reaction 3							
CRHTS3b	-1077.79305	21.7	0.04335	0.00014	90.9	-1076.57967	-1076.58169
HTS3b	-1077.78474	20.2	0.04094	-0.00281	92.1	-1076.57383	-1076.57565
CPHTS3b	-1077.85983	24.1	0.04884	0.00048	101.4	-1076.65418	-1076.65666
CRHTS3a	-1077.79305	21.7	0.04335	0.00014	90.9	-1076.57967	-1076.58169
HTS3a	-1077.78654	20.4	0.04098	-0.00170	89.8	-1076.57726	-1076.57912
CPHTS3a	-1077.85983	24.1	0.04884	0.00048	101.4	-1076.65418	-1076.65666
Reaction 5							
CRHTS5a	-1077.79547	23.5	0.04691	-0.00065	100.1	-1076.58563	
HTS5a	-1077.77894	20.3	0.04056	-0.00178	89.1	-1076.57060	
CPHTS5a	-1077.81290	21.9	0.04411	0.00132	95.6	-1076.60484	
Reaction 6							
CRHTS6a	-1077.79798	24.0	0.04705	0.00332	92.0	-1076.58934	
HTS6a	-1077.78020	20.8	0.04173	-0.00159	91.2	-1076.57360	
CPHTS6a	-1077.80806	23.5	0.04686	0.00012	98.4	-1076.59813	
Reaction 8							
CRHTS8a	-1077.80919	22.9	0.04584	0.00044	95.6	-1076.60044	
HTS8a	-1077.78110	18.7	0.03843	-0.00484	91.1	-1076.57638	
CPHTS8a	-1077.82450	20.6	0.04339	-0.00635	104.7	-1076.62095	
CRHTS8b	-1077.80919	22.9	0.04584	0.00044	95.6	-1076.60044	
HTS8b	-1077.78180	18.8	0.03843	-0.00461	90.6	-1076.57724	
CPHTS8b	-1077.82449	20.6	0.04339	-0.00635	104.7	-1076.62095	

In table S6 we have collected the detail of the rate constants computed for all elementary reactions R1 to R12. Almost all rate constant calculations have been computed with conventional and variational transition state theory (VTST). However, there are few cases, either no relevant of because the reaction path is very flat and we could not get enough s points, in which only conventional transition state theory has been applied (TST). In general, conventional transition state theory rate constants are up to twice greater than variational transition state theory calculated values, although in some cases the differences raise up to five times.

Table S6. Calculated rate constants for all elementary reactions investigated in this work, computed at different temperatures (T in Kelvin). Keq stands for equilibrium constants (in $\text{cm}^3 \cdot \text{molecule}^{-1}$); ktst and kcvt stand for conventional rate constants and canonic variational rate constants (in s^{-1}), and kt stands for total rate constants (in $\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$). When applied, tunn stands for the tunneling correction, and for all VTST calculations, the s range considered is included as footnote.

Reactions starting by HSSH + OH

FTS1a

T	Keq	ktst	kcvt	kt
220.00	5.50e-22	4.930e+02	4.87e+02	2.68e-19
230.00	4.11e-22	1.220e+03	1.20e+03	4.94e-19
240.00	3.16e-22	2.780e+03	2.74e+03	8.67e-19
250.00	2.49e-22	5.940e+03	5.86e+03	1.46e-18
260.00	2.00e-22	1.200e+04	1.18e+04	2.36e-18
270.00	1.64e-22	2.290e+04	2.26e+04	3.71e-18
280.00	1.37e-22	4.170e+04	4.11e+04	5.63e-18
290.00	1.16e-22	7.290e+04	7.19e+04	8.33e-18
298.00	1.02e-22	1.110e+05	1.09e+05	1.12e-17
300.00	9.93e-23	1.230e+05	1.21e+05	1.20e-17
310.00	8.62e-23	2.000e+05	1.97e+05	1.70e-17
320.00	7.56e-23	3.150e+05	3.10e+05	2.34e-17

S :0.149,0.2988, 0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.589, 4.499, at both sides of the IRC

FTS1b

# T	Keq	ktst	kcvt	kt
220.00	5.50e-22	4.93e+02	4.87e+02	2.68e-19
230.00	4.11e-22	1.22e+03	1.20e+03	4.94e-19
240.00	3.16e-22	2.78e+03	2.74e+03	8.67e-19
250.00	2.49e-22	5.94e+03	5.86e+03	1.46e-18
260.00	2.00e-22	1.20e+04	1.18e+04	2.36e-18
270.00	1.64e-22	2.29e+04	2.26e+04	3.71e-18

280.00	1.37e-22	4.17e+04	4.11e+04	5.63e-18
290.00	1.16e-22	7.29e+04	7.19e+04	8.33e-18
298.00	1.02e-22	1.11e+05	1.09e+05	1.12e-17
300.00	9.93e-23	1.23e+05	1.21e+05	1.20e-17
310.00	8.62e-23	2.00e+05	1.97e+05	1.70e-17
320.00	7.56e-23	3.15e+05	3.10e+05	2.34e-17

S :0.149,0.2988, 0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.589, 4.499, at both sides of the IRC

BTS1a

# T	Keq	ktst	kcvt	kt
220.00	5.50e-22	1.40e+09	1.22e+09	6.70e-13
230.00	4.11e-22	1.65e+09	1.44e+09	5.92e-13
240.00	3.16e-22	1.92e+09	1.67e+09	5.28e-13
250.00	2.49e-22	2.20e+09	1.92e+09	4.78e-13
260.00	2.00e-22	2.50e+09	2.17e+09	4.35e-13
270.00	1.64e-22	2.81e+09	2.43e+09	3.99e-13
280.00	1.37e-22	3.12e+09	2.71e+09	3.71e-13
290.00	1.16e-22	3.45e+09	2.98e+09	3.45e-13
298.00	1.02e-22	3.71e+09	3.21e+09	3.29e-13
300.00	9.93e-23	3.78e+09	3.27e+09	3.25e-13
310.00	8.62e-23	4.11e+09	3.55e+09	3.06e-13
320.00	7.56e-23	4.46e+09	3.84e+09	2.90e-13

S :0.149,0.2988, 0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.589, 4.499, at both sides of the IRC

BTS1b

# T	Keq	ktst	kcvt	kt
220.00	5.50e-22	1.40e+09	1.22e+09	6.70e-13
230.00	4.11e-22	1.65e+09	1.44e+09	5.92e-13
240.00	3.16e-22	1.92e+09	1.67e+09	5.28e-13
250.00	2.49e-22	2.20e+09	1.92e+09	4.78e-13
260.00	2.00e-22	2.50e+09	2.17e+09	4.35e-13
270.00	1.64e-22	2.81e+09	2.43e+09	3.99e-13
280.00	1.37e-22	3.12e+09	2.71e+09	3.71e-13
290.00	1.16e-22	3.45e+09	2.98e+09	3.45e-13
298.00	1.02e-22	3.71e+09	3.21e+09	3.29e-13
300.00	9.93e-23	3.78e+09	3.27e+09	3.25e-13
310.00	8.62e-23	4.11e+09	3.55e+09	3.06e-13
320.00	7.56e-23	4.46e+09	3.84e+09	2.90e-13

S :0.149,0.2988, 0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.589, 4.499, at both sides of the IRC

HTS3a

# T	Keq	tunn	ktst	kcvt:	kt
220.00	5.50e-22	1.47	9.57e+10	8.07e+10	6.54e-11
230.00	4.11e-22	1.41	1.14e+11	9.91e+10	5.76e-11
240.00	3.16e-22	1.37	1.33e+11	1.20e+11	5.19e-11
250.00	2.49e-22	1.33	1.53e+11	1.42e+11	4.71e-11

260.00	2.00e-22	0.81	1.75e+11	1.63e+11	2.65e-11
270.00	1.64e-22	0.81	1.98e+11	1.84e+11	2.45e-11
280.00	1.37e-22	0.81	2.22e+11	2.06e+11	2.27e-11
290.00	1.16e-22	0.80	2.47e+11	2.29e+11	2.13e-11
298.00	1.02e-22	0.80	2.67e+11	2.48e+11	2.04e-11
300.00	9.93e-23	0.81	2.73e+11	2.52e+11	2.02e-11
310.00	8.62e-23	0.80	2.99e+11	2.77e+11	1.91e-11
320.00	7.56e-23	0.80	3.26e+11	3.01e+11	1.83e-11

S= 0.204, 0.409, 0.818, 1.225, 1.634, 2.053, 2.452, 2.816, 3. 271, 3.925 at both sides of the IRC

HTS3b

# T	Keq	tunn	ktst	kcvt	kt
220.00	6.92e-22	1.30	1.19e+11	9.82e+10	8.86e-11
230.00	5.79e-22	1.27	1.23e+11	1.05e+11	7.70e-11
240.00	4.93e-22	1.23	1.28e+11	1.11e+11	6.76e-11
250.00	4.27e-22	1.21	1.32e+11	1.17e+11	6.02e-11
260.00	3.75e-22	1.19	1.35e+11	1.22e+11	5.44e-11
270.00	3.33e-22	1.16	1.39e+11	1.28e+11	4.97e-11
280.00	3.00e-22	1.15	1.42e+11	1.33e+11	4.59e-11
290.00	2.72e-22	1.13	1.45e+11	1.38e+11	4.25e-11
298.00	2.54e-22	0.82	1.47e+11	1.40e+11	2.92e-11
300.00	2.50e-22	0.82	1.48e+11	1.41e+11	2.87e-11
310.00	2.31e-22	0.82	1.50e+11	1.43e+11	2.70e-11
320.00	2.15e-22	0.82	1.53e+11	1.45e+11	2.55e-11

S=0124, 0.207, 0.623, 0.830, 1.038, 1,243, 1.451, 2.074, 2.489, 2.904, 3.734, 4.564, 6.224 , - 0124, -0.207,- 0.623, -0.830, 1.038, -1,243, -1.451, -2.074, -2.489

PTS3a

# T	Keq	tunn	ktst	kcvt	kt
220.00	5.50e-22	1067.57	3.74e+06	3.70e+06	2.17e-12
230.00	4.11e-22	653.97	6.36e+06	6.30e+06	1.69e-12
240.00	3.16e-22	422.55	1.03e+07	1.02e+07	1.36e-12
250.00	2.49e-22	281.88	1.62e+07	1.60e+07	1.12e-12
260.00	2.00e-22	195.45	2.44e+07	2.42e+07	9.48e-13
270.00	1.64e-22	140.23	3.56e+07	3.53e+07	8.13e-13
280.00	1.37e-22	103.59	5.07e+07	5.02e+07	7.12e-13
290.00	1.16e-22	78.19	7.03e+07	6.97e+07	6.31e-13
298.00	1.02e-22	63.71	8.98e+07	8.90e+07	5.80e-13
300.00	9.93e-23	60.63	9.53e+07	9.45e+07	5.69e-13
310.00	8.62e-23	47.70	1.27e+08	1.26e+08	5.18e-13
320.00	7.56e-23	38.54	1.65e+08	1.64e+08	4.78e-13

S= 0.150, 0.300, 0.600, -0.150, -0.300, -0.600, -0.900, -1.500

Reverse BTS1a

# T	Keq	ktst	kcvt	kt
220.00	1.01e-22	4.17e+03	3.69e+03	3.72e-19
230.00	7.04e-23	1.08e+04	9.49e+03	6.68e-19
240.00	5.07e-23	2.57e+04	2.26e+04	1.15e-18

250.00	3.76e-23	5.72e+04	5.03e+04	1.89e-18
260.00	2.86e-23	1.20e+05	1.05e+05	3.01e-18
270.00	2.23e-23	2.38e+05	2.09e+05	4.66e-18
280.00	1.77e-23	4.51e+05	3.94e+05	6.98e-18
290.00	1.43e-23	8.16e+05	7.14e+05	1.02e-17
298.00	1.22e-23	1.28e+06	1.11e+06	1.36e-17
300.00	1.18e-23	1.42e+06	1.24e+06	1.46e-17
310.00	9.82e-24	2.39e+06	2.09e+06	2.05e-17
320.00	8.30e-24	3.89e+06	3.39e+06	2.81e-17

S :0.149,0.2988, 0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.589, 4.499, at both sides of the IRC

Reverse BTS1b

# T	Keq	ktst	kcvt	kt
220.00	1e-222	4.17e+03	3.69e+03	3.72e-19
230.00	7e-232	1.08e+04	9.49e+03	6.68e-19
240.00	5e-232	2.57e+04	2.26e+04	1.15e-18
250.00	4e-232	5.72e+04	5.03e+04	1.89e-18
260.00	3e-232	1.20e+05	1.05e+05	3.01e-18
270.00	2e-232	2.38e+05	2.09e+05	4.66e-18
280.00	2e-232	4.51e+05	3.94e+05	6.98e-18
290.00	1e-232	8.16e+05	7.14e+05	1.02e-17
298.00	1e-232	1.28e+06	1.11e+06	1.36e-17
300.00	1e-232	1.42e+06	1.24e+06	1.46e-17
310.00	1e-232	2.39e+06	2.09e+06	2.05e-17
320.00	8e-242	3.89e+06	3.39e+06	2.81e-17

S :0.149,0.2988, 0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.589, 4.499, at both sides of the IRC

HTS5a

# T	Keq	tunn	ktst	kcvt: kt	
220.00	8.55e-21	576.20	1.24e+03	6.89e+02	3.40e-15
230.00	5.13e-21	353.12	3.44e+03	1.92e+03	3.48e-15
240.00	3.22e-21	230.14	8.72e+03	4.91e+03	3.63e-15
250.00	2.10e-21	156.41	2.06e+04	1.17e+04	3.84e-15
260.00	1.42e-21	111.92	4.54e+04	2.60e+04	4.13e-15
270.00	9.89e-22	82.72	9.47e+04	5.44e+04	4.45e-15
280.00	7.09e-22	63.24	1.87e+05	1.08e+05	4.84e-15
290.00	5.21e-22	49.03	3.54e+05	2.06e+05	5.26e-15
298.00	4.14e-22	41.14	5.71e+05	3.33e+05	5.67e-15
300.00	3.92e-22	39.57	6.42e+05	3.74e+05	5.80e-15
310.00	3.00e-22	32.16	1.12e+06	6.56e+05	6.34e-15
320.00	2.35e-22	26.76	1.89e+06	1.11e+06	6.97e-15

S=0.156, 0.313, 0.469, 0.625, 0.938, 1.250, 1.813, -0.156, -0.313, -0.469, -0.625, -0.938, -1.250, 1.813, -2.500, -3.438, -4.376

HTS5b

# T	Keq	tunn	ktst	kcvt	kt	
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220.00	3.39e-21	371.76	2.90e+03	2.16e+03	2.73e-15
230.00	2.15e-21	233.74	7.61e+03	5.69e+03	2.86e-15
240.00	1.42e-21	155.07	1.84e+04	1.38e+04	3.04e-15
250.00	9.73e-22	107.99	4.16e+04	3.13e+04	3.29e-15
260.00	6.87e-22	78.31	8.83e+04	6.64e+04	3.57e-15
270.00	4.99e-22	58.58	1.77e+05	1.34e+05	3.92e-15
280.00	3.72e-22	45.31	3.39e+05	2.56e+05	4.32e-15
290.00	2.83e-22	35.90	6.20e+05	4.68e+05	4.76e-15
298.00	2.31e-22	30.35	9.77e+05	7.38e+05	5.18e-15
300.00	2.20e-22	29.13	1.09e+06	8.24e+05	5.29e-15
310.00	1.74e-22	24.00	1.85e+06	1.40e+06	5.86e-15
320.00	1.40e-22	20.13	3.04e+06	2.30e+06	6.50e-15

S=0.156, 0.313, 0.469, 0.625, 0.938, 1.250, 1.813, 2.503, 3.441, 4,380, -0.156, -0.313, -0.469, -0.625, -0.938, -1.250, 1.813, -2.500, -3.438,-4.376

HTS6a

# T	Keq	tunn	ktst	kcvt: kt	
220.00	3.35e-23	1.32	1.41e+10	5.89e+09	2.61e-13
230.00	2.78e-23	1.27	1.77e+10	7.78e+09	2.76e-13
240.00	2.36e-23	1.24	2.17e+10	1.00e+10	2.92e-13
250.00	2.03e-23	1.20	2.63e+10	1.27e+10	3.08e-13
260.00	1.77e-23	1.17	3.15e+10	1.57e+10	3.26e-13
270.00	1.57e-23	1.15	3.71e+10	1.92e+10	3.45e-13
280.00	1.40e-23	1.13	4.32e+10	2.31e+10	3.64e-13
290.00	1.27e-23	1.10	4.99e+10	2.75e+10	3.84e-13
298.00	1.18e-23	1.09	5.56e+10	3.12e+10	4.00e-13
300.00	1.16e-23	1.09	5.70e+10	3.22e+10	4.05e-13
310.00	1.06e-23	1.07	6.47e+10	3.75e+10	4.26e-13
320.00	9.85e-24	1.06	7.28e+10	4.31e+10	4.49e-13

S= 0.155, 0.308, 0.462, 0.615, 0.922, 1.230, 1.784, 2.461, 2.923, -0.155, -0.308, -0.462, -0.615, -0.922, -1.230, -1.784, -2.461, -3.380, -4.300

HTS6b

T	Keq	tunn	ktst	kcvt	kt	
220.00	8.55e-21	1.43	3.39e+07	1.68e+07	2.06e-13	
230.00	5.13e-21	1.37	6.02e+07	3.13e+07	2.20e-13	
240.00	3.22e-21	1.32	1.02e+08	5.55e+07	2.35e-13	
250.00	2.10e-21	1.27	1.66e+08	9.39e+07	2.50e-13	
260.00	1.42e-21	1.23	2.60e+08	1.53e+08	2.67e-13	
270.00	9.89e-22	1.20	3.95e+08	2.40e+08	2.84e-13	
280.00	7.09e-22	1.16	5.83e+08	3.65e+08	3.01e-13	
290.00	5.21e-22	1.14	8.38e+08	5.39e+08	3.20e-13	
298.00	4.14e-22	1.12	1.10e+09	7.23e+08	3.36e-13	
300.00	3.92e-22	1.12	1.18e+09	7.76e+08	3.40e-13	
310.00	3.00e-22	1.10	1.62e+09	1.09e+09	3.61e-13	
320.00	2.35e-22	1.08	2.18e+09	1.51e+09	3.83e-13	

S= 0.155, 0.308, 0.462, 0.615, 0.922, 1.230, 1.784, 2.460, 3.380,4.302, -0.155, -0.308, -0.462, -0.615, -0.922, -1.230, -1.784, -2.461, -3.380, -4.300

Reactions starting by HSSCH₃ + OH

BTS1a

T	Keq	ktst	kt
220.00	3.68e-22	5.34e+10	1.97e-11
230.00	3.21e-22	5.43e+10	1.75e-11
240.00	2.84e-22	5.50e+10	1.56e-11
250.00	2.55e-22	5.56e+10	1.42e-11
260.00	2.32e-22	5.62e+10	1.30e-11
270.00	2.12e-22	5.65e+10	1.20e-11
280.00	1.97e-22	5.69e+10	1.12e-11
290.00	1.83e-22	5.72e+10	1.05e-11
298.00	1.74e-22	5.74e+10	1.00e-11
300.00	1.72e-22	5.75e+10	9.91e-12
310.00	1.63e-22	5.76e+10	9.39e-12
320.00	1.55e-22	5.78e+10	8.96e-12

Calculated at conventional TST only

Reverse BTS1a

T	Keq	kTST	kt
220.00	1.53e-23	8.43e+04	1.29e-18
230.00	1.11e-23	1.86e+05	2.06e-18
240.00	8.30e-24	3.86e+05	3.20e-18
250.00	6.38e-24	7.54e+05	4.81e-18
260.00	5.03e-24	1.40e+06	7.04e-18
270.00	4.04e-24	2.49e+06	1.01e-17
280.00	3.31e-24	4.25e+06	1.41e-17
290.00	2.76e-24	6.99e+06	1.93e-17
298.00	2.41e-24	1.02e+07	2.46e-17
300.00	2.34e-24	1.11e+07	2.59e-17
310.00	2.00e-24	1.72e+07	3.45e-17
320.00	1.74e-24	2.60e+07	4.52e-17

Calculated at conventional TST only

BTS1b

T	Keq	ktst	kt
220.00	5.05e-22	3.46e+11	1.75e-10
230.00	4.05e-22	3.42e+11	1.39e-10
240.00	3.33e-22	3.38e+11	1.12e-10
250.00	2.78e-22	3.35e+11	9.30e-11
260.00	2.36e-22	3.31e+11	7.82e-11
270.00	2.04e-22	3.27e+11	6.67e-11
280.00	1.78e-22	3.24e+11	5.77e-11
290.00	1.58e-22	3.20e+11	5.05e-11
298.00	1.44e-22	3.18e+11	4.58e-11
300.00	1.41e-22	3.17e+11	4.47e-11

310.00	1.27e-22	3.14e+11	3.99e-11
320.00	1.16e-22	3.11e+11	3.60e-11

Calculated at conventional TST only

Reverse BTS1B

# T	Keq	kTST	kt
220.00	3.12e-24	3.77e+06	1.18e-17
230.00	2.40e-24	7.02e+06	1.69e-17
240.00	1.90e-24	1.24e+07	2.35e-17
250.00	1.54e-24	2.11e+07	3.24e-17
260.00	1.27e-24	3.42e+07	4.33e-17
270.00	1.06e-24	5.38e+07	5.72e-17
280.00	9.08e-25	8.18e+07	7.43e-17
290.00	7.86e-25	1.21e+08	9.51e-17
298.00	7.06e-25	1.62e+08	1.14e-16
300.00	6.89e-25	1.74e+08	1.20e-16
310.00	6.10e-25	2.45e+08	1.50e-16
320.00	5.46e-25	3.38e+08	1.85e-16

Calculated at conventional TST only

FTS1a

T	Keq	ktst	kcvt	kt
220.00	5.05e-22	7.43e+00	5.93e+00	2.99e-21
230.00	4.05e-22	2.08e+01	1.67e+01	6.77e-21
240.00	3.33e-22	5.33e+01	4.30e+01	1.43e-20
250.00	2.78e-22	1.27e+02	1.03e+02	2.86e-20
260.00	2.36e-22	2.81e+02	2.29e+02	5.41e-20
270.00	2.04e-22	5.88e+02	4.81e+02	9.81e-20
280.00	1.78e-22	1.16e+03	9.56e+02	1.70e-19
290.00	1.58e-22	2.20e+03	1.81e+03	2.86e-19
298.00	1.44e-22	3.54e+03	2.93e+03	4.22e-19
300.00	1.41e-22	3.98e+03	3.29e+03	4.64e-19
310.00	1.27e-22	6.91e+03	5.73e+03	7.29e-19
320.00	1.16e-22	1.16e+04	9.65e+03	1.12e-18

S= 0.285, 0.571, 1.142, 1.714, 2.855, 3.997, 4.568, 5.170,,6.851, 7.708, -0.428, -0.856,-1.713, -2.569, -4.283, -5.995, -6.852, -8.563

FTS1b

T	Keq	ktst	kcvt	kt
220.00	3.68e-22	6.53e+04	6.33e+04	2.33e-17
230.00	3.21e-22	1.17e+05	1.14e+05	3.66e-17
240.00	2.84e-22	2.00e+05	1.94e+05	5.52e-17
250.00	2.55e-22	3.27e+05	3.17e+05	8.09e-17
260.00	2.32e-22	5.13e+05	4.98e+05	1.15e-16
270.00	2.12e-22	7.78e+05	7.56e+05	1.61e-16
280.00	1.97e-22	1.14e+06	1.11e+06	2.18e-16
290.00	1.83e-22	1.63e+06	1.59e+06	2.92e-16
298.00	1.74e-22	2.14e+06	2.08e+06	3.63e-16
300.00	1.72e-22	2.28e+06	2.22e+06	3.83e-16

310.00	1.63e-22	3.11e+06	3.03e+06	4.94e-16
320.00	1.55e-22	4.16e+06	4.05e+06	6.28e-16

S= 0.374 0.747, 1.494, 2.242, 3.736, 5.230, 5.753, -0.374, -0.742, -1.494, -2.242, -3.736, -5.230, -5.997, -6.724

BTS2a

T	Keq	ktst	kcvt	kt
220.00	9.80e-20	1.42e+11	1.19e+11	1.17e-08
230.00	5.78e-20	1.56e+11	1.31e+11	7.58e-09
240.00	3.58e-20	1.70e+11	1.42e+11	5.08e-09
250.00	2.31e-20	1.84e+11	1.53e+11	3.53e-09
260.00	1.54e-20	1.97e+11	1.65e+11	2.54e-09
270.00	1.06e-20	2.11e+11	1.76e+11	1.87e-09
280.00	7.56e-21	2.25e+11	1.87e+11	1.41e-09
290.00	5.51e-21	2.38e+11	1.97e+11	1.09e-09
298.00	4.36e-21	2.48e+11	2.06e+11	8.97e-10
300.00	4.12e-21	2.51e+11	2.08e+11	8.56e-10
310.00	3.14e-21	2.64e+11	2.18e+11	6.84e-10
320.00	2.44e-21	2.76e+11	2.28e+11	5.55e-10

S= 0.144, 0.294, 0.593, 0.893, 1.492, 2.096, 2.390, 2.989, 3.579, 4,452, -0.145, -0.295, -0.594, -0.894, -1.494, -2.094, -2.394, -2.994, -3.594, -4.493

Reverse BTS2a

# T	Keq	ktst	kt
220.00	3.87e-20	1.88e+03	7.27e-17
230.00	2.25e-20	4.76e+03	1.07e-16
240.00	1.38e-20	1.12e+04	1.54e-16
250.00	8.80e-21	2.45e+04	2.16e-16
260.00	5.83e-21	5.05e+04	2.94e-16
270.00	3.99e-21	9.87e+04	3.94e-16
280.00	2.82e-21	1.84e+05	5.18e-16
290.00	2.04e-21	3.29e+05	6.71e-16
298.00	1.60e-21	5.10e+05	8.18e-16
300.00	1.51e-21	5.66e+05	8.57e-16
310.00	1.15e-21	9.41e+05	1.08e-15
320.00	8.87e-22	1.52e+06	1.35e-15

Calculated at conventional TST only

BTS2b

T	Keq	ktst	kcvt	kt
220.00	9.44e-19	1.86e+11	1.39e+11	1.31e-07
230.00	4.85e-19	2.08e+11	1.55e+11	7.52e-08
240.00	2.64e-19	2.30e+11	1.71e+11	4.52e-08
250.00	1.51e-19	2.53e+11	1.87e+11	2.83e-08
260.00	9.08e-20	2.75e+11	2.03e+11	1.84e-08
270.00	5.67e-20	2.98e+11	2.19e+11	1.24e-08
280.00	3.67e-20	3.21e+11	2.35e+11	8.62e-09
290.00	2.45e-20	3.43e+11	2.51e+11	6.15e-09

298.00	1.81e-20	3.61e+11	2.63e+11	4.77e-09
300.00	1.69e-20	3.66e+11	2.66e+11	4.49e-09
310.00	1.19e-20	3.88e+11	2.82e+11	3.36e-09
320.00	8.61e-21	4.10e+11	2.97e+11	2.56e-09

S= 0.144, 0.294, 0.593, 0.893, 1.492, 2.096, 2.390, 2.989, 3.579, 4,452, -0.145, -0.295, -0.594, -0.894, -1.494, -2.094, -2.394, -2.994, -3.594, -4.493

Reverse BTS2b

# T	Keq	ktst	kt
220.00	2.87e-21	3.10e+05	8.89e-16
230.00	2.02e-21	5.78e+05	1.16e-15
240.00	1.46e-21	1.02e+06	1.49e-15
250.00	1.09e-21	1.73e+06	1.89e-15
260.00	8.39e-22	2.80e+06	2.35e-15
270.00	6.59e-22	4.39e+06	2.89e-15
280.00	5.27e-22	6.65e+06	3.51e-15
290.00	4.30e-22	9.80e+06	4.21e-15
298.00	3.69e-22	1.31e+07	4.84e-15
300.00	3.56e-22	1.41e+07	5.02e-15
310.00	2.99e-22	1.97e+07	5.89e-15
320.00	2.55e-22	2.71e+07	6.90e-15

Calculated at conventional TST only

FTS2a

T	Keq	ktst	kcvt	kt
220.00	9.34e-19	8.27e+03	3.24e+03	3.03e-15
230.00	4.81e-19	1.93e+04	7.72e+03	3.71e-15
240.00	2.62e-19	4.19e+04	1.71e+04	4.48e-15
250.00	1.50e-19	8.55e+04	3.56e+04	5.36e-15
260.00	9.03e-20	1.65e+05	7.00e+04	6.32e-15
270.00	5.65e-20	3.04e+05	1.31e+05	7.40e-15
280.00	3.66e-20	5.35e+05	2.34e+05	8.56e-15
290.00	2.45e-20	9.06e+05	4.01e+05	9.81e-15
298.00	1.81e-20	1.35e+06	6.01e+05	1.09e-14
300.00	1.68e-20	1.48e+06	6.63e+05	1.12e-14
310.00	1.19e-20	2.34e+06	1.06e+06	1.26e-14
320.00	8.61e-21	3.61e+06	1.65e+06	1.42e-14

S=0.285, 0.571, 1.142, 1.713, 2.855, 3.997, 4.568, 5.710, 6.852, 7.708, -0.428, -0.756, -1,713, -2.569, -4.282, -5.995, -6.851, -8.563.

FTS2b

T	Keq	ktst	kcvt	kt
220.00	3.58e-20	4.17e+08	1.87e+08	6.70e-12
230.00	2.05e-20	6.22e+08	2.90e+08	5.94e-12
240.00	1.23e-20	9.00e+08	4.34e+08	5.33e-12
250.00	7.70e-21	1.26e+09	6.29e+08	4.84e-12
260.00	5.00e-21	1.73e+09	8.84e+08	4.42e-12
270.00	3.36e-21	2.31e+09	1.21e+09	4.07e-12

280.00	2.33e-21	3.03e+09	1.63e+09	3.80e-12
290.00	1.66e-21	3.90e+09	2.14e+09	3.54e-12
298.00	1.28e-21	4.71e+09	2.63e+09	3.37e-12
300.00	1.21e-21	4.94e+09	2.76e+09	3.33e-12

S= 0.531, 1.063, 2.127, 3.190, -0.531, -1.063, -2.127, -3.190, -4.784, -4.889

HTS3a

T	Keq	tunn	ktst	kcvt	kt
220.00	9.78e-19	6.05	4.35e+07	4.28e+07	2.53e-10
230.00	5.02e-19	5.36	7.33e+07	7.22e+07	1.94e-10
240.00	2.73e-19	4.81	1.18e+08	1.16e+08	1.53e-10
250.00	1.57e-19	4.34	1.84e+08	1.81e+08	1.23e-10
260.00	9.39e-20	3.97	2.76e+08	2.72e+08	1.01e-10
270.00	5.86e-20	3.66	4.02e+08	3.96e+08	8.50e-11
280.00	3.79e-20	3.39	5.69e+08	5.61e+08	7.20e-11
290.00	2.53e-20	3.17	7.88e+08	7.77e+08	6.23e-11
298.00	1.87e-20	3.01	1.01e+09	9.93e+08	5.60e-11
300.00	1.74e-20	2.98	1.07e+09	1.05e+09	5.45e-11
310.00	1.23e-20	2.81	1.42e+09	1.40e+09	4.83e-11
320.00	8.88e-21	2.66	1.85e+09	1.83e+09	4.32e-11

S=0.154, 0.307, 0.461, 0.617, 0.773, 0.987, 1.085, 1.239, 1.,387, 1,535, 2.312, 3.090, 4.024, -0.155, -0.311, -0467, -0.622

HTS3b

T	Keq	tunn	ktst	kcvt	kt
220.00	5.05e-22	1.27	1.59e+12	1.59e+12	1.02e-09
230.00	4.05e-22	1.25	1.67e+12	1.67e+12	8.43e-10
240.00	3.33e-22	1.23	1.76e+12	1.75e+12	7.15e-10
250.00	2.78e-22	1.21	1.84e+12	1.84e+12	6.17e-10
260.00	2.36e-22	1.19	1.91e+12	1.91e+12	5.39e-10
270.00	2.04e-22	1.18	1.99e+12	1.99e+12	4.77e-10
280.00	1.78e-22	1.17	2.06e+12	2.06e+12	4.28e-10
290.00	1.58e-22	1.15	2.13e+12	2.13e+12	3.87e-10
298.00	1.44e-22	1.14	2.18e+12	2.18e+12	3.59e-10
300.00	1.41e-22	1.14	2.19e+12	2.19e+12	3.53e-10
310.00	1.27e-22	1.13	2.26e+12	2.26e+12	3.26e-10
320.00	1.16e-22	1.12	2.32e+12	2.32e+12	3.02e-10

S= 0.210, 0.421, 0.841, 1.261, 2.103, 2.944, 3.366, 4.207, 5.048, -0.210, -0.421, -0.842, -1.263, -2.105, -2.946, -3.367, -4.209, -5.051, -6.313.

PTS3a

T	Keq	tunn	ktst	kcvt	kt
220.00	9.78e-19	169.66	4.05e+08	3.56e+08	5.91e-08
230.00	5.02e-19	121.61	5.91e+08	5.23e+08	3.19e-08
240.00	2.73e-19	89.91	8.36e+08	7.43e+08	1.83e-08
250.00	1.57e-19	67.96	1.15e+09	1.03e+09	1.10e-08
260.00	9.39e-20	53.19	1.54e+09	1.38e+09	6.89e-09
270.00	5.86e-20	42.20	2.02e+09	1.82e+09	4.50e-09
280.00	3.79e-20	34.32	2.60e+09	2.34e+09	3.04e-09

290.00	2.53e-20	28.22	3.29e+09	2.97e+09	2.12e-09
298.00	1.87e-20	24.45	3.92e+09	3.55e+09	1.63e-09
300.00	1.74e-20	23.65	4.09e+09	3.70e+09	1.52e-09
310.00	1.23e-20	20.04	5.01e+09	4.55e+09	1.12e-09
320.00	8.88e-21	17.21	6.07e+09	5.52e+09	8.44e-10

S=0.153, 0.307, 0.614, 0.920, 1.534, 2.147, 2.454, 3.067, 3.681, 4.602, -0.154, -0.307, -0.614, -0.920, -1.540, -2.147, -2.454, -3.068, -3.681

PTS3b

T	Keq	tunn	ktst	kcvt	kt
220.00	9.88e-19	843.75	1.91e+06	1.60e+06	1.33e-09
230.00	5.08e-19	506.67	3.56e+06	3.00e+06	7.72e-10
240.00	2.76e-19	320.22	6.31e+06	5.34e+06	4.73e-10
250.00	1.58e-19	212.79	1.07e+07	9.07e+06	3.06e-10
260.00	9.49e-20	147.30	1.73e+07	1.48e+07	2.07e-10
270.00	5.93e-20	105.15	2.71e+07	2.33e+07	1.45e-10
280.00	3.83e-20	77.75	4.11e+07	3.55e+07	1.06e-10
290.00	2.56e-20	59.16	6.06e+07	5.24e+07	7.94e-11
298.00	1.89e-20	48.36	8.10e+07	7.03e+07	6.44e-11
300.00	1.76e-20	45.96	8.69e+07	7.55e+07	6.11e-11
310.00	1.24e-20	36.70	1.22e+08	1.06e+08	4.84e-11
320.00	8.99e-21	29.79	1.67e+08	1.46e+08	3.91e-11

S= S=0.153, 0.307, 0.614, 0.920, 1.534, 2.147, 2.454, 3.067, 3.681, 4.602, -0.154, -0.307, -0.614, -0.920, -1.540, -2.147, -2.454, -3.068, -3.681

HTS11a

T	Keq	tunn	ktst	kcvt	kt
220.00	5.51e-22	5.50	1.03e+11	1.03e+10	3.12e-11
230.00	4.31e-22	4.82	1.22e+11	1.35e+10	2.81e-11
240.00	3.45e-22	4.29	1.43e+11	1.73e+10	2.56e-11
250.00	2.82e-22	3.87	1.65e+11	2.18e+10	2.38e-11
260.00	2.34e-22	3.51	1.88e+11	2.70e+10	2.23e-11
270.00	1.98e-22	3.22	2.13e+11	3.29e+10	2.10e-11
280.00	1.70e-22	2.99	2.39e+11	3.94e+10	2.01e-11
290.00	1.48e-22	2.80	2.67e+11	4.68e+10	1.94e-11
298.00	1.33e-22	2.65	2.89e+11	5.32e+10	1.88e-11
300.00	1.30e-22	2.62	2.95e+11	5.49e+10	1.87e-11
310.00	1.16e-22	2.48	3.25e+11	6.37e+10	1.83e-11
320.00	1.04e-22	2.35	3.55e+11	7.33e+10	1.78e-11

S= 0.157, 0.314, 0.629, 0.943, 1.572, 2.201, 2.515, 3.144, 3.772, 4.716, -0.157, -0.314, -0.629, -0.942, -1.572, -2.200, -2.515, -3.143, -3.772, -4.716

HTS11b

T	Keq	tunn	ktst	kcvt	kt
220.00	1.30e-21	4.69	1.19e+10	9.76e+08	5.95e-12
230.00	1.01e-21	4.13	1.54e+10	1.42e+09	5.95e-12
240.00	8.09e-22	3.72	1.95e+10	1.99e+09	6.00e-12
250.00	6.60e-22	3.38	2.43e+10	2.73e+09	6.09e-12
260.00	5.49e-22	3.10	2.97e+10	3.64e+09	6.20e-12

270.00	4.63e-22	2.87	3.59e+10	4.77e+09	6.35e-12
280.00	3.97e-22	2.68	4.28e+10	6.12e+09	6.51e-12
290.00	3.45e-22	2.52	5.05e+10	7.73e+09	6.73e-12
298.00	3.11e-22	2.40	5.71e+10	9.21e+09	6.87e-12
300.00	3.03e-22	2.38	5.89e+10	9.60e+09	6.91e-12
310.00	2.69e-22	2.25	6.80e+10	1.18e+10	7.16e-12
320.00	2.41e-22	2.16	7.80e+10	1.42e+10	7.40e-12

S= 0.157, 0.315, 0.631, 0.947, 1.578, 2.209, 2.524, 3.156, 3.787,4.733, at both sides of the IRC

HTS5a

T	Keq	tunn	ktst	kcvt	kt
220.00	1.97e-20	547619.05	3.81e+02	3.78e+02	4.08e-12
230.00	1.26e-20	224509.80	1.03e+03	1.02e+03	2.89e-12
240.00	8.41e-21	100395.26	2.55e+03	2.53e+03	2.14e-12
250.00	5.81e-21	48287.67	5.88e+03	5.84e+03	1.64e-12
260.00	4.15e-21	24645.67	1.27e+04	1.27e+04	1.30e-12
270.00	3.05e-21	13436.29	2.61e+04	2.59e+04	1.06e-12
280.00	2.29e-21	7658.73	5.07e+04	5.04e+04	8.85e-13
290.00	1.77e-21	4578.44	9.43e+04	9.37e+04	7.57e-13
298.00	1.45e-21	3127.52	1.50e+05	1.49e+05	6.77e-13
300.00	1.39e-21	2850.30	1.68e+05	1.67e+05	6.60e-13
310.00	1.11e-21	1833.33	2.89e+05	2.88e+05	5.86e-13
320.00	9.02e-22	1221.29	4.81e+05	4.79e+05	5.28e-13

S= 0.156, 0.312, 0.624, 0.936, 1.560, 2.138, 2.496, 3.120, 3.744, 4.680, at both sides of the IRC

HTS5b

T	Keq	tunn	ktst	kcvt	kt
220.00	1.97e-20	125179.86	1.48e+01	1.39e+01	3.43e-14
230.00	1.26e-20	59540.23	4.63e+01	4.35e+01	3.27e-14
240.00	8.41e-21	30403.23	1.31e+02	1.24e+02	3.17e-14
250.00	5.81e-21	16584.62	3.44e+02	3.25e+02	3.13e-14
260.00	4.15e-21	9557.52	8.36e+02	7.91e+02	3.14e-14
270.00	3.05e-21	5777.78	1.90e+03	1.80e+03	3.17e-14
280.00	2.29e-21	3624.68	4.09e+03	3.89e+03	3.23e-14
290.00	1.77e-21	2367.76	8.34e+03	7.94e+03	3.32e-14
298.00	1.45e-21	1727.94	1.43e+04	1.36e+04	3.42e-14
300.00	1.39e-21	1600.00	1.62e+04	1.55e+04	3.44e-14
310.00	1.11e-21	1110.73	3.03e+04	2.89e+04	3.56e-14
320.00	9.02e-22	792.31	5.44e+04	5.20e+04	3.72e-14

S= 0.156, 0.312, 0.624, 0.936, 1.560, 2.138, 2.496, 3.120, 3.744, 4.680, at both sides of the IRC

HTS6a

T	Keq	tunn	ktst	kcvt	kt
220.00	5.24e-22	13.20	4.25e+08	3.22e+08	2.22e-12
230.00	4.04e-22	11.15	6.09e+08	4.68e+08	2.11e-12

240.00	3.21e-22	9.58	8.46e+08	6.59e+08	2.02e-12
250.00	2.60e-22	8.36	1.14e+09	9.02e+08	1.96e-12
260.00	2.16e-22	7.36	1.51e+09	1.21e+09	1.92e-12
270.00	1.82e-22	6.58	1.96e+09	1.58e+09	1.89e-12
280.00	1.56e-22	5.94	2.50e+09	2.02e+09	1.87e-12
290.00	1.35e-22	5.41	3.12e+09	2.55e+09	1.87e-12
298.00	1.22e-22	5.03	3.70e+09	3.04e+09	1.87e-12
300.00	1.19e-22	4.95	3.85e+09	3.17e+09	1.87e-12
310.00	1.06e-22	4.58	4.69e+09	3.89e+09	1.89e-12
320.00	9.54e-23	4.23	5.64e+09	4.71e+09	1.90e-12

S= 0.156, 0.312, 0.624, 0.936, 1.560, 2.138, 2.496, 3.120, 3.744, 4.680, at both sides of the IRC

HTS6b

T	Keq	tunn	ktst	kcvt	kt
220.00	2.61e-20	4.12	1.78e+05	1.73e+05	1.86e-14
230.00	1.67e-20	3.72	3.58e+05	3.47e+05	2.15e-14
240.00	1.11e-20	3.36	6.77e+05	6.57e+05	2.46e-14
250.00	7.69e-21	3.10	1.22e+06	1.18e+06	2.81e-14
260.00	5.48e-21	2.86	2.09e+06	2.04e+06	3.20e-14
270.00	4.02e-21	2.68	3.46e+06	3.37e+06	3.63e-14
280.00	3.03e-21	2.51	5.52e+06	5.38e+06	4.09e-14
290.00	2.33e-21	2.38	8.52e+06	8.32e+06	4.61e-14
298.00	1.92e-21	2.29	1.18e+07	1.15e+07	5.04e-14
300.00	1.83e-21	2.26	1.28e+07	1.25e+07	5.16e-14
310.00	1.46e-21	2.15	1.87e+07	1.83e+07	5.76e-14
320.00	1.19e-21	2.06	2.67e+07	2.62e+07	6.41e-14

S= 0.156, 0.312, 0.624, 0.936, 1.560, 2.138, 2.496, 3.120, 3.744, 4.680, at both sides of the IRC

HTS8a

T	Keq	tunn	ktst	kcvt	kt
220.00	1.94e-17	38.53	4.99e+02	4.36e+02	3.26e-13
230.00	8.40e-18	29.27	1.40e+03	1.23e+03	3.02e-13
240.00	3.91e-18	23.01	3.59e+03	3.19e+03	2.87e-13
250.00	1.94e-18	18.67	8.55e+03	7.66e+03	2.77e-13
260.00	1.02e-18	15.41	1.91e+04	1.72e+04	2.70e-13
270.00	5.62e-19	12.99	4.02e+04	3.64e+04	2.66e-13
280.00	3.24e-19	11.12	8.01e+04	7.31e+04	2.63e-13
290.00	1.94e-19	9.64	1.53e+05	1.40e+05	2.63e-13
298.00	1.33e-19	8.73	2.48e+05	2.28e+05	2.64e-13
300.00	1.21e-19	8.48	2.78e+05	2.57e+05	2.64e-13
310.00	7.78e-20	7.57	4.89e+05	4.52e+05	2.66e-13
320.00	5.15e-20	6.79	8.30e+05	7.70e+05	2.69e-13

S= 0.156, 0.312, 0.624, 0.936, 1.560, 2.138, 2.496, 3.120, 3.744, 4.680, at both sides of the IRC

HTS8b

T	Keq	tunn	ktst	kcvt	kt
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220.00	1.68e-18	14.43	8.37e+03	5.66e+02	1.38e-14
230.00	8.24e-19	11.35	2.04e+04	1.55e+03	1.45e-14
240.00	4.29e-19	9.28	4.61e+04	3.91e+03	1.56e-14
250.00	2.36e-19	7.81	9.77e+04	9.16e+03	1.69e-14
260.00	1.36e-19	6.72	1.96e+05	2.01e+04	1.84e-14
270.00	8.21e-20	5.83	3.73e+05	4.17e+04	2.00e-14
280.00	5.14e-20	5.17	6.78e+05	8.20e+04	2.18e-14
290.00	3.33e-20	4.64	1.18e+06	1.54e+05	2.38e-14
298.00	2.41e-20	4.27	1.80e+06	2.48e+05	2.56e-14
300.00	2.23e-20	4.21	2.00e+06	2.78e+05	2.61e-14
310.00	1.53e-20	3.85	3.25e+06	4.83e+05	2.85e-14
320.00	1.08e-20	3.54	5.14e+06	8.10e+05	3.10e-14

S= 0.156, 0.312, 0.624, 0.936, 1.560, 2.138, 2.496, 3.120, 3.744, 4.680, at both sides of the IRC

Reactions starting by HSSNH₂ + OH

BTS1a

T	Keq	kTST	kt
220.00	3.18e-22	4.59e+10	1.46e-11
230.00	2.80e-22	4.62e+10	1.29e-11
240.00	2.50e-22	4.65e+10	1.16e-11
250.00	2.26e-22	4.66e+10	1.05e-11
260.00	2.07e-22	4.67e+10	9.65e-12
270.00	1.91e-22	4.68e+10	8.92e-12
280.00	1.78e-22	4.68e+10	8.32e-12
290.00	1.67e-22	4.68e+10	7.80e-12
298.00	1.59e-22	4.68e+10	7.45e-12
300.00	1.57e-22	4.68e+10	7.36e-12
310.00	1.50e-22	4.67e+10	6.99e-12
320.00	1.43e-22	4.67e+10	6.68e-12

Conventional TST only

Reverse-BTS1a

T	Keq	ktst	kt
220.00	4.98e-22	4.11e-07	2.04e-28
230.00	3.29e-22	2.48e-06	8.16e-28
240.00	2.26e-22	1.28e-05	2.90e-27
250.00	1.61e-22	5.84e-05	9.41e-27
260.00	1.18e-22	2.36e-04	2.79e-26
270.00	8.90e-23	8.63e-04	7.68e-26
280.00	6.87e-23	2.87e-03	1.97e-25
290.00	5.41e-23	8.80e-03	4.76e-25
298.00	4.53e-23	2.04e-02	9.24e-25
300.00	4.34e-23	2.50e-02	1.09e-24
310.00	3.55e-23	6.66e-02	2.36e-24
320.00	2.94e-23	1.67e-01	4.91e-24

Conventional TST only

Reverse-BTS1b

T	Keq	ktst	kt
220.00	4.98e-22	1.53e-08	7.61e-30
230.00	3.29e-22	1.08e-07	3.55e-29
240.00	2.26e-22	6.45e-07	1.46e-28
250.00	1.61e-22	3.35e-06	5.40e-28
260.00	1.18e-22	1.53e-05	1.81e-27
270.00	8.90e-23	6.26e-05	5.57e-27
280.00	6.87e-23	2.32e-04	1.59e-26
290.00	5.41e-23	7.85e-04	4.25e-26
298.00	4.53e-23	1.96e-03	8.88e-26
300.00	4.34e-23	2.45e-03	1.06e-25
310.00	3.55e-23	7.11e-03	2.52e-25
320.00	2.94e-23	1.93e-02	5.68e-25

Conventional TST only

BTS1b

T	Keq	ktST	kt
220.00	3.53e-22	1.46e+09	5.15e-13
230.00	2.72e-22	1.96e+09	5.33e-13
240.00	2.15e-22	2.57e+09	5.53e-13
250.00	1.74e-22	3.30e+09	5.73e-13
260.00	1.43e-22	4.16e+09	5.94e-13
270.00	1.19e-22	5.16e+09	6.17e-13
280.00	1.01e-22	6.30e+09	6.39e-13
290.00	8.72e-23	7.59e+09	6.62e-13
298.00	7.80e-23	8.74e+09	6.81e-13
300.00	7.59e-23	9.04e+09	6.86e-13
310.00	6.68e-23	1.07e+10	7.14e-13
320.00	5.93e-23	1.24e+10	7.35e-13

Conventional TST only

FTS1a

T	Keq	ktst	kcvt	kt
220.00	3.18e-22	5.15e+06	5.07e+06	1.61e-15
230.00	2.80e-22	8.05e+06	7.93e+06	2.22e-15
240.00	2.50e-22	1.21e+07	1.19e+07	2.97e-15
250.00	2.26e-22	1.76e+07	1.74e+07	3.93e-15
260.00	2.07e-22	2.49e+07	2.46e+07	5.08e-15
270.00	1.91e-22	3.42e+07	3.38e+07	6.44e-15
280.00	1.78e-22	4.60e+07	4.54e+07	8.06e-15
290.00	1.67e-22	6.05e+07	5.97e+07	9.95e-15
298.00	1.59e-22	7.42e+07	7.33e+07	1.17e-14
300.00	1.57e-22	7.80e+07	7.70e+07	1.21e-14
310.00	1.50e-22	9.89e+07	9.77e+07	1.46e-14
320.00	1.43e-22	1.23e+08	1.22e+08	1.74e-14

S= 0.244, 0.488, 0.977, 1.466, 2.447,3.420, 3.908, 4.885,5.816,6.253, at both sides of the IRC

FTS1b

T	Keq	ktst	kcvt	kt
220.00	3.53e-22	8.42e+01	7.36e+01	2.60e-20
230.00	2.72e-22	2.13e+02	1.87e+02	5.09e-20
240.00	2.15e-22	4.98e+02	4.38e+02	9.42e-20
250.00	1.74e-22	1.09e+03	9.57e+02	1.66e-19
260.00	1.43e-22	2.23e+03	1.97e+03	2.81e-19
270.00	1.19e-22	4.34e+03	3.84e+03	4.59e-19
280.00	1.01e-22	8.04e+03	7.13e+03	7.23e-19
290.00	8.72e-23	1.43e+04	1.27e+04	1.11e-18
298.00	7.80e-23	2.19e+04	1.95e+04	1.52e-18
300.00	7.59e-23	2.43e+04	2.17e+04	1.65e-18
310.00	6.68e-23	4.01e+04	3.58e+04	2.39e-18
320.00	5.93e-23	6.41e+04	5.72e+04	3.39e-18

S= 0.274, 0.548, 1.095, 1.643, 2.3879, 3.834, 4.3812, 5.468, 6.572,7.013 , at both sides of the IRC

BTS2a

T	Keq	ktst	kcvt	kt
220.00	3.38e-19	3.13e+10	2.87e+10	9.69e-09
230.00	1.78e-19	3.86e+10	3.54e+10	6.29e-09
240.00	9.88e-20	4.67e+10	4.29e+10	4.24e-09
250.00	5.78e-20	5.56e+10	5.12e+10	2.96e-09
260.00	3.53e-20	6.53e+10	6.03e+10	2.13e-09
270.00	2.25e-20	7.58e+10	7.01e+10	1.57e-09
280.00	1.48e-20	8.71e+10	8.06e+10	1.19e-09
290.00	1.00e-20	9.90e+10	9.18e+10	9.21e-10
298.00	7.52e-21	1.09e+11	1.01e+11	7.59e-10
300.00	7.01e-21	1.12e+11	1.04e+11	7.29e-10
310.00	5.02e-21	1.25e+11	1.16e+11	5.82e-10
320.00	3.68e-21	1.39e+11	1.29e+11	4.75e-10

S= 0.147, 0.296, 0.595, 0.895,1.494, 2.092, 2.393, 3.588, 4.4.86, -0.147, -0.296, -0.595, -0.895,-1.494, -2.092, -2.395, -2.995, - 3.595, -4.495

Reverse-BTS2a

T	Keq	ktst	kt
220.00	5.64e-21	5.50e-02	3.10e-22
230.00	3.49e-21	2.16e-01	7.53e-22
240.00	2.25e-21	7.59e-01	1.71e-21
250.00	1.51e-21	2.41e+00	3.65e-21
260.00	1.05e-21	7.01e+00	7.36e-21
270.00	7.51e-22	1.89e+01	1.42e-20
280.00	5.52e-22	4.72e+01	2.60e-20
290.00	4.15e-22	1.11e+02	4.61e-20
298.00	3.36e-22	2.12e+02	7.12e-20

300.00	3.19e-22	2.47e+02	7.88e-20
310.00	2.50e-22	5.22e+02	1.30e-19
320.00	1.99e-22	1.05e+03	2.09e-19

Conventional TST only

Reverse-BTS2b

T	Keq	ktst	kt
220.00	5.64e-21	3.09e-03	1.74e-23
230.00	3.49e-21	1.40e-02	4.88e-23
240.00	2.25e-21	5.56e-02	1.25e-22
250.00	1.51e-21	1.99e-01	3.01e-22
260.00	1.05e-21	6.43e-01	6.75e-22
270.00	7.51e-22	1.91e+00	1.43e-21
280.00	5.52e-22	5.26e+00	2.90e-21
290.00	4.15e-22	1.35e+01	5.60e-21
298.00	3.36e-22	2.74e+01	9.20e-21
300.00	3.19e-22	3.26e+01	1.04e-20
310.00	2.50e-22	7.42e+01	1.85e-20
320.00	1.99e-22	1.61e+02	3.21e-20

Conventional TST only

BTS2b

# T	Keq	ktst	kcvt	kt
220.00	6.33e-20	1.08e+10	1.02e+10	6.45e-10
230.00	3.74e-20	1.35e+10	1.28e+10	4.79e-10
240.00	2.32e-20	1.66e+10	1.57e+10	3.65e-10
250.00	1.50e-20	2.01e+10	1.91e+10	2.87e-10
260.00	1.01e-20	2.39e+10	2.27e+10	2.29e-10
270.00	6.99e-21	2.81e+10	2.67e+10	1.87e-10
280.00	4.99e-21	3.27e+10	3.11e+10	1.55e-10
290.00	3.65e-21	3.76e+10	3.57e+10	1.30e-10
298.00	2.90e-21	4.17e+10	3.97e+10	1.15e-10
300.00	2.74e-21	4.27e+10	4.07e+10	1.11e-10
310.00	2.10e-21	4.82e+10	4.59e+10	9.62e-11
320.00	1.63e-21	5.40e+10	5.14e+10	8.40e-11

S= 0.147, 0.296, 0.595, 0.895, 1.494, 2.092, 2.393, 3.588, 4.4.86, -0.147, -0.296, -0.595, -0.895, -1.494, -2.092, -2.395, -2.995, -3.595, -4.495

FTS2a

T	Keq	ktst	kcvt	kt
220.00	1.07e-18	1.51e+06	1.35e+06	1.44e-12
230.00	5.34e-19	2.71e+06	2.42e+06	1.29e-12
240.00	2.83e-19	4.63e+06	4.15e+06	1.18e-12
250.00	1.58e-19	7.57e+06	6.80e+06	1.08e-12
260.00	9.28e-20	1.19e+07	1.07e+07	9.93e-13
270.00	5.67e-20	1.81e+07	1.64e+07	9.30e-13
280.00	3.60e-20	2.68e+07	2.43e+07	8.74e-13
290.00	2.36e-20	3.85e+07	3.49e+07	8.24e-13
298.00	1.72e-20	5.06e+07	4.59e+07	7.90e-13

300.00	1.59e-20	5.40e+07	4.91e+07	7.83e-13
310.00	1.11e-20	7.41e+07	6.75e+07	7.48e-13
320.00	7.88e-21	9.97e+07	9.09e+07	7.16e-13

S= 0.242, 0.484, 0.968, 1.453, 2.421, 3.389, 3.873, 4.836, -0.242, -0.484, -0.968, -1.453, -2.421, -3.389, -3.873, -4.836, -5.807, -7.256

FTS2b

T	Keq	ktst	kcvt	kt
220.00	9.69e-18	1.10e+05	6.72e+04	6.51e-13
230.00	4.31e-18	2.35e+05	1.45e+05	6.25e-13
240.00	2.06e-18	4.69e+05	2.92e+05	6.00e-13
250.00	1.04e-18	8.88e+05	5.59e+05	5.83e-13
260.00	5.58e-19	1.60e+06	1.02e+06	5.70e-13
270.00	3.14e-19	2.76e+06	1.77e+06	5.56e-13
280.00	1.84e-19	4.59e+06	2.95e+06	5.43e-13
290.00	1.12e-19	7.35e+06	4.76e+06	5.35e-13
298.00	7.76e-20	1.05e+07	6.82e+06	5.29e-13
300.00	7.10e-20	1.14e+07	7.43e+06	5.28e-13
310.00	4.63e-20	1.72e+07	1.13e+07	5.23e-13
320.00	3.10e-20	2.54e+07	1.67e+07	5.18e-13

S=0.264, 0.5238, 1.055, 2.638, 3.694, 4.221, 5.278, -0.264, -0.5238, -1.055, -2.638, -3.694, -4.221, -5.278, -6.327, -7.907

HTS3a

T	Keq	tun	ktst	kcvt	kt
220.00	1.55e-21	0.67	2.51e+11	2.18e+11	2.28e-10
230.00	1.14e-21	0.67	2.81e+11	2.45e+11	1.87e-10
240.00	8.58e-22	0.68	3.12e+11	2.71e+11	1.57e-10
250.00	6.65e-22	0.68	3.43e+11	2.98e+11	1.34e-10
260.00	5.27e-22	0.68	3.74e+11	3.25e+11	1.17e-10
270.00	4.27e-22	0.68	4.06e+11	3.53e+11	1.03e-10
280.00	3.51e-22	0.68	4.37e+11	3.80e+11	9.13e-11
290.00	2.94e-22	0.69	4.69e+11	4.07e+11	8.23e-11
298.00	2.57e-22	0.69	4.94e+11	4.28e+11	7.60e-11
300.00	2.49e-22	0.69	5.01e+11	4.34e+11	7.46e-11
310.00	2.14e-22	0.69	5.32e+11	4.60e+11	6.84e-11
320.00	1.86e-22	0.69	5.63e+11	4.87e+11	6.30e-11

S= 0.-207, 0.413, 0.827, 1.238, 2.066, 2.893, 3.305, 4.131, 4.,957, 6.197, at both sides of the IRC

HTS3b

T	Keq	tun	ktst	kcvt	kt
220.00	9.69e-18	1.28	2.24e+07	1.70e+07	2.11e-10
230.00	4.31e-18	1.25	4.20e+07	3.30e+07	1.78e-10
240.00	2.06e-18	1.22	7.48e+07	6.07e+07	1.53e-10
250.00	1.04e-18	1.20	1.27e+08	1.06e+08	1.32e-10
260.00	5.58e-19	1.17	2.08e+08	1.79e+08	1.17e-10
270.00	3.14e-19	0.69	3.29e+08	2.85e+08	6.15e-11
280.00	1.84e-19	0.69	5.02e+08	4.36e+08	5.55e-11

290.00	1.12e-19	0.69	7.45e+08	6.46e+08	5.04e-11
298.00	7.76e-20	0.70	1.00e+09	8.69e+08	4.70e-11
300.00	7.10e-20	0.70	1.08e+09	9.34e+08	4.62e-11
310.00	4.63e-20	0.70	1.52e+09	1.32e+09	4.27e-11
320.00	3.10e-20	0.70	2.10e+09	1.82e+09	3.97e-11

S= 0.248, 0.497, 0.994, 1.489, 2.484, 3.478, 3.975, 4.969, 5.963, -0.248, -0.497, -0.994, -1.489, -2.484, -3.478, -3.129

PTS3a

T	Keq	tun	ktst	kcvt	kt
220.00	3.38e-19	119.08	2.75e+07	2.62e+07	1.05e-09
230.00	1.78e-19	81.24	4.41e+07	4.21e+07	6.07e-10
240.00	9.88e-20	57.45	6.80e+07	6.51e+07	3.70e-10
250.00	5.78e-20	42.27	1.01e+08	9.70e+07	2.37e-10
260.00	3.53e-20	32.07	1.46e+08	1.40e+08	1.59e-10
270.00	2.25e-20	25.10	2.05e+08	1.96e+08	1.10e-10
280.00	1.48e-20	20.04	2.80e+08	2.69e+08	7.96e-11
290.00	1.00e-20	16.36	3.75e+08	3.60e+08	5.91e-11
298.00	7.52e-21	14.08	4.66e+08	4.49e+08	4.75e-11
300.00	7.01e-21	13.59	4.91e+08	4.73e+08	4.51e-11
310.00	5.02e-21	11.51	6.33e+08	6.10e+08	3.52e-11
320.00	3.68e-21	9.90	8.02e+08	7.73e+08	2.82e-11

S=0.154, 0.397, 0.614, 0.921, 1.536, 2.150, 2.458, 3.072, 3.686, 4.609, at both sides of the IRC.

HTS5a

T	Keq	tunn	ktst	kcvt	kt
220.00	2.23e-19	1706.98	2.53e-06	2.15e-06	8.20e-22
230.00	1.11e-19	951.61	1.46e-05	1.24e-05	1.32e-21
240.00	5.92e-20	562.90	7.26e-05	6.20e-05	2.07e-21
250.00	3.32e-20	352.21	3.17e-04	2.72e-04	3.18e-21
260.00	1.95e-20	232.08	1.24e-03	1.06e-03	4.79e-21
270.00	1.20e-20	158.78	4.37e-03	3.76e-03	7.14e-21
280.00	7.61e-21	113.22	1.41e-02	1.21e-02	1.04e-20
290.00	5.01e-21	82.60	4.19e-02	3.62e-02	1.50e-20
298.00	3.67e-21	65.94	9.52e-02	8.22e-02	1.99e-20
300.00	3.41e-21	62.60	1.16e-01	1.00e-01	2.13e-20
310.00	2.38e-21	48.46	3.01e-01	2.60e-01	2.99e-20
320.00	1.70e-21	38.21	7.34e-01	6.36e-01	4.13e-20

S= 0.157, 0.315, 0.630, 0.944, 1.574, 2.204, 2.519, 3.148, 3.778, 4.722, at both sides of the IRC

HTS5b

T	Keq	tunn	ktst	kcvt	kt
220.00	5.59e-20	8576.92	4.52e-10	1.04e-10	4.98e-26
230.00	3.15e-20	4235.81	3.93e-09	9.16e-10	1.22e-25
240.00	1.87e-20	2274.74	2.86e-08	6.77e-09	2.88e-25
250.00	1.16e-20	1309.86	1.77e-07	4.26e-08	6.49e-25
260.00	7.53e-21	798.28	9.56e-07	2.33e-07	1.40e-24

270.00	5.04e-21	516.07	4.55e-06	1.12e-06	2.92e-24
280.00	3.49e-21	346.47	1.94e-05	4.82e-06	5.83e-24
290.00	2.48e-21	241.49	7.48e-05	1.88e-05	1.13e-23
298.00	1.93e-21	185.63	2.06e-04	5.22e-05	1.87e-23
300.00	1.81e-21	174.89	2.64e-04	6.69e-05	2.12e-23
310.00	1.35e-21	129.22	8.59e-04	2.19e-04	3.83e-23
320.00	1.03e-21	98.35	2.60e-03	6.68e-04	6.78e-23

S= 0.157, 0.315, 0.630, 0.944, 1.574, 2.204, 2.519, 3.148, 3.778, 4,722, at both sides of the IRC

HTS6a

T	Keq	tunn	ktst	kcvt	kt
220.00	7.23e-21	14.29	1.12e-03	1.12e-03	1.16e-22
230.00	4.42e-21	11.85	4.93e-03	4.93e-03	2.58e-22
240.00	2.83e-21	10.05	1.91e-02	1.91e-02	5.43e-22
250.00	1.88e-21	8.65	6.66e-02	6.66e-02	1.08e-21
260.00	1.30e-21	7.54	2.11e-01	2.11e-01	2.06e-21
270.00	9.21e-22	6.68	6.12e-01	6.12e-01	3.76e-21
280.00	6.72e-22	5.97	1.65e+00	1.65e+00	6.62e-21
290.00	5.03e-22	5.40	4.15e+00	4.15e+00	1.13e-20
298.00	4.06e-22	5.00	8.30e+00	8.30e+00	1.68e-20
300.00	3.85e-22	4.91	9.82e+00	9.81e+00	1.86e-20
310.00	3.01e-22	4.50	2.20e+01	2.20e+01	2.98e-20
320.00	2.39e-22	4.17	4.69e+01	4.68e+01	4.67e-20

S=0.153, 0.305, 0.6210, 0.915, 1.526, 2.136, 2.441, 3.052, 3.662, 4.578, at both sides of the IRC

HTS6b

T	Keq	tunn	ktst	kcvt	kt
220.00	7.23e-21	6.69	9.87e-03	9.81e-03	4.75e-22
230.00	4.42e-21	5.77	3.98e-02	3.95e-02	1.01e-21
240.00	2.83e-21	5.06	1.43e-01	1.42e-01	2.03e-21
250.00	1.88e-21	4.51	4.61e-01	4.59e-01	3.89e-21
260.00	1.30e-21	4.06	1.36e+00	1.36e+00	7.15e-21
270.00	9.21e-22	3.69	3.72e+00	3.71e+00	1.26e-20
280.00	6.72e-22	3.41	9.46e+00	9.41e+00	2.16e-20
290.00	5.03e-22	3.17	2.26e+01	2.24e+01	3.57e-20
298.00	4.06e-22	2.99	4.33e+01	4.31e+01	5.24e-20
300.00	3.85e-22	2.95	5.07e+01	5.05e+01	5.74e-20
310.00	3.01e-22	2.77	1.08e+02	1.08e+02	9.00e-20
320.00	2.39e-22	2.62	2.21e+02	2.19e+02	1.37e-19

S=0.153, 0.305, 0.6210, 0.915, 1.526, 2.136, 2.441, 3.052, 3.662, 4.578, at both sides of the IRC

HTS8a

T	Keq	tunn	ktst	kcvt	kt
220.00	5.92e-18	2.41	2.20e+03	1.44e+03	2.06e-14
230.00	2.67e-18	2.10	5.98e+03	3.95e+03	2.22e-14
240.00	1.29e-18	1.89	1.50e+04	9.93e+03	2.43e-14

250.00	6.65e-19	1.72	3.48e+04	2.32e+04	2.66e-14
260.00	3.61e-19	1.59	7.59e+04	5.09e+04	2.92e-14
270.00	2.05e-19	1.50	1.56e+05	1.05e+05	3.22e-14
280.00	1.22e-19	1.40	3.06e+05	2.07e+05	3.53e-14
290.00	7.50e-20	1.33	5.73e+05	3.88e+05	3.87e-14
298.00	5.22e-20	1.28	9.17e+05	6.23e+05	4.17e-14
300.00	4.79e-20	1.27	1.03e+06	6.99e+05	4.25e-14
310.00	3.15e-20	1.22	1.78e+06	1.21e+06	4.66e-14
320.00	2.13e-20	1.18	2.97e+06	2.03e+06	5.10e-14

S= 0.161, 0.323, 0.645, 0.968, 1.613, 2.259, 2.581, 3.227, 3.872, 4.840, at both sides of the IRC

HTS8b

T	Keq	tunn	ktst	kcvt	kt
220.00	5.92e-18	5.11	1.16e-12	6.10e-13	1.85e-29
230.00	2.67e-18	3.15	5.18e-12	2.75e-12	2.32e-29
240.00	1.29e-18	2.48	2.04e-11	1.09e-11	3.49e-29
250.00	6.65e-19	2.13	7.23e-11	3.90e-11	5.52e-29
260.00	3.61e-19	1.91	2.32e-10	1.27e-10	8.72e-29
270.00	2.05e-19	1.76	6.86e-10	3.77e-10	1.36e-28
280.00	1.22e-19	1.63	1.88e-09	1.04e-09	2.07e-28
290.00	7.50e-20	1.54	4.80e-09	2.67e-09	3.09e-28
298.00	5.22e-20	1.48	9.73e-09	5.43e-09	4.20e-28
300.00	4.79e-20	1.46	1.15e-08	6.45e-09	4.52e-28
310.00	3.15e-20	1.40	2.63e-08	1.47e-08	6.49e-28
320.00	2.13e-20	1.34	5.68e-08	3.20e-08	9.15e-28

S= 0.161, 0.323, 0.645, 0.968, 1.613, 2.259, 2.581, 3.227, 3.872, 4.840, at both sides of the IRC

Reactions starting by HSSCOOH + OH

BTS1a

T	Keq	ktst	kt
220.00	1.21e-23	2.26e+10	2.73e-13
230.00	1.18e-23	2.34e+10	2.78e-13
240.00	1.17e-23	2.42e+10	2.82e-13
250.00	1.15e-23	2.49e+10	2.88e-13
260.00	1.15e-23	2.56e+10	2.93e-13
270.00	1.14e-23	2.62e+10	2.99e-13
280.00	1.14e-23	2.67e+10	3.05e-13
290.00	1.15e-23	2.72e+10	3.11e-13
298.00	1.15e-23	2.75e+10	3.17e-13
300.00	1.15e-23	2.76e+10	3.18e-13
310.00	1.16e-23	2.80e+10	3.25e-13
320.00	1.17e-23	2.84e+10	3.32e-13

Conventional TST only

Reverse-BTS1a

T	Keq	ktst	kt
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220.00	6.51e-24	2.22e+03	1.44e-20
230.00	4.62e-24	5.67e+03	2.62e-20
240.00	3.39e-24	1.34e+04	4.54e-20
250.00	2.56e-24	2.97e+04	7.61e-20
260.00	1.99e-24	6.17e+04	1.23e-19
270.00	1.57e-24	1.22e+05	1.92e-19
280.00	1.27e-24	2.29e+05	2.92e-19
290.00	1.05e-24	4.13e+05	4.33e-19
298.00	9.09e-25	6.43e+05	5.85e-19
300.00	8.79e-25	7.16e+05	6.29e-19
310.00	7.46e-25	1.20e+06	8.95e-19
320.00	6.42e-25	1.94e+06	1.25e-18

Conventional TST only

BTS1b

T	Keq	ktst	kt
220.00	2.95e-22	1.32e+10	3.89e-12
230.00	2.52e-22	1.41e+10	3.55e-12
240.00	2.19e-22	1.49e+10	3.27e-12
250.00	1.94e-22	1.57e+10	3.04e-12
260.00	1.73e-22	1.64e+10	2.84e-12
270.00	1.56e-22	1.71e+10	2.68e-12
280.00	1.43e-22	1.78e+10	2.54e-12
290.00	1.32e-22	1.84e+10	2.42e-12
298.00	1.24e-22	1.89e+10	2.35e-12
300.00	1.22e-22	1.90e+10	2.32e-12
310.00	1.14e-22	1.96e+10	2.24e-12
320.00	1.08e-22	2.01e+10	2.17e-12

Conventional TST only

Reverse-BTS1b

T	Keq	ktst	kt
220.00	6.51e-24	2.22e+03	1.44e-20
230.00	4.62e-24	5.67e+03	2.62e-20
240.00	3.39e-24	1.34e+04	4.54e-20
250.00	2.56e-24	2.97e+04	7.61e-20
260.00	1.99e-24	6.17e+04	1.23e-19
270.00	1.57e-24	1.22e+05	1.92e-19
280.00	1.27e-24	2.29e+05	2.92e-19
290.00	1.05e-24	4.13e+05	4.33e-19
298.00	9.09e-25	6.43e+05	5.85e-19
300.00	8.79e-25	7.16e+05	6.29e-19
310.00	7.46e-25	1.20e+06	8.95e-19
320.00	6.42e-25	1.94e+06	1.25e-18

Conventional TST only

FTS1a

T	Keq	ktst	kcvt	kt
220.00	5.54e-20	6.79e-03	6.75e-03	3.74e-22

230.00	3.32e-20	2.58e-02	2.57e-02	8.54e-22
240.00	2.09e-20	8.76e-02	8.71e-02	1.82e-21
250.00	1.36e-20	2.69e-01	2.68e-01	3.65e-21
260.00	9.21e-21	7.58e-01	7.55e-01	6.95e-21
270.00	6.43e-21	1.98e+00	1.97e+00	1.27e-20
280.00	4.61e-21	4.80e+00	4.78e+00	2.20e-20
290.00	3.39e-21	1.10e+01	1.09e+01	3.70e-20
298.00	2.70e-21	2.04e+01	2.03e+01	5.47e-20
300.00	2.55e-21	2.37e+01	2.36e+01	6.02e-20
310.00	1.96e-21	4.86e+01	4.84e+01	9.48e-20
320.00	1.53e-21	9.53e+01	9.49e+01	1.45e-19

S= 0.149, 0.299, 0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.599, 4.499, at both sides of the IRC

FTS1b

T	Keq	ktst	kcvt	kt
220.00	5.77e-23	1.66e+05	7.43e+04	4.29e-18
230.00	4.96e-23	2.95e+05	1.34e+05	6.65e-18
240.00	4.34e-23	4.99e+05	2.30e+05	9.97e-18
250.00	3.84e-23	8.08e+05	3.78e+05	1.45e-17
260.00	3.45e-23	1.26e+06	5.96e+05	2.05e-17
270.00	3.13e-23	1.90e+06	9.07e+05	2.84e-17
280.00	2.86e-23	2.77e+06	1.34e+06	3.84e-17
290.00	2.65e-23	3.95e+06	1.92e+06	5.08e-17
298.00	2.50e-23	5.14e+06	2.52e+06	6.30e-17
300.00	2.46e-23	5.48e+06	2.69e+06	6.63e-17
310.00	2.31e-23	7.44e+06	3.67e+06	8.48e-17
320.00	2.18e-23	9.90e+06	4.92e+06	1.07e-16

S= 0.149, 0.299, 0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.599, 4.499, at both sides of the IRC

BTS2a

T	Keq	ktst	kt
220.00	6.80e-23	5.76e+07	3.92e-15
230.00	5.69e-23	8.24e+07	4.69e-15
240.00	4.85e-23	1.14e+08	5.53e-15
250.00	4.20e-23	1.55e+08	6.51e-15
260.00	3.69e-23	2.04e+08	7.53e-15
270.00	3.28e-23	2.63e+08	8.63e-15
280.00	2.95e-23	3.34e+08	9.87e-15
290.00	2.68e-23	4.16e+08	1.12e-14
298.00	2.50e-23	4.91e+08	1.23e-14
300.00	2.46e-23	5.11e+08	1.26e-14
310.00	2.28e-23	6.19e+08	1.41e-14
320.00	2.12e-23	7.40e+08	1.57e-14

Conventional TST only

FTS2a

T	Keq	ktst	kcvt	kt
220.00	3.60e-22	2.34e+02	2.14e+02	7.70e-20
230.00	2.69e-22	5.76e+02	5.26e+02	1.42e-19
240.00	2.07e-22	1.31e+03	1.20e+03	2.49e-19
250.00	1.63e-22	2.80e+03	2.56e+03	4.18e-19
260.00	1.32e-22	5.62e+03	5.14e+03	6.77e-19
270.00	1.08e-22	1.07e+04	9.81e+03	1.06e-18
280.00	9.03e-23	1.95e+04	1.79e+04	1.62e-18
290.00	7.65e-23	3.40e+04	3.12e+04	2.39e-18
298.00	6.77e-23	5.16e+04	4.74e+04	3.21e-18
300.00	6.57e-23	5.71e+04	5.24e+04	3.44e-18
310.00	5.72e-23	9.27e+04	8.52e+04	4.87e-18
320.00	5.02e-23	1.46e+05	1.34e+05	6.73e-18

S= 0.149, 0.299, 0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.599, 4.499, at both sides of the IRC

FTS2b

T	Keq	ktst	kcvt	kt
220.00	6.80e-23	1.50e+04	1.35e+04	9.18e-19
230.00	5.69e-23	2.96e+04	2.66e+04	1.51e-18
240.00	4.85e-23	5.53e+04	4.98e+04	2.41e-18
250.00	4.20e-23	9.80e+04	8.83e+04	3.71e-18
260.00	3.69e-23	1.66e+05	1.50e+05	5.53e-18
270.00	3.28e-23	2.71e+05	2.44e+05	8.01e-18
280.00	2.95e-23	4.25e+05	3.83e+05	1.13e-17
290.00	2.68e-23	6.47e+05	5.83e+05	1.57e-17
298.00	2.50e-23	8.86e+05	7.99e+05	2.00e-17
300.00	2.46e-23	9.56e+05	8.62e+05	2.12e-17
310.00	2.28e-23	1.38e+06	1.24e+06	2.82e-17
320.00	2.12e-23	1.94e+06	1.75e+06	3.71e-17

S= 0.149, 0.299, 0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.599, 4.499, at both sides of the IRC

HTS3a

T	Keq	tunn	ktst	kcvt	kt
220.00	4.71e-20	1.72	7.63e+08	6.09e+08	4.95e-11
230.00	2.83e-20	1.64	1.10e+09	9.12e+08	4.24e-11
240.00	1.78e-20	1.56	1.54e+09	1.32e+09	3.66e-11
250.00	1.16e-20	1.49	2.10e+09	1.86e+09	3.22e-11
260.00	7.86e-21	1.43	2.79e+09	2.55e+09	2.87e-11
270.00	5.48e-21	1.38	3.64e+09	3.41e+09	2.58e-11
280.00	3.94e-21	1.33	4.66e+09	4.48e+09	2.35e-11
290.00	2.90e-21	0.78	5.86e+09	5.68e+09	1.28e-11
298.00	2.30e-21	0.77	6.97e+09	6.75e+09	1.20e-11
300.00	2.18e-21	0.77	7.26e+09	7.04e+09	1.19e-11
310.00	1.67e-21	0.77	8.88e+09	8.60e+09	1.11e-11
320.00	1.31e-21	0.76	1.07e+10	1.04e+10	1.04e-11

S= 0.190, 0.381, 0.762, 1.141, 1.190, 2.665, 3.046, 3.807, 4.566, 5.704, at both sides of the IRC

HTS3b

T	Keq	tunn	ktst	kcvt	kt
220.00	4.71e-20	2.33	1.16e+11	6.58e+10	7.21e-09
230.00	2.83e-20	2.18	1.21e+11	7.17e+10	4.41e-09
240.00	1.78e-20	2.05	1.26e+11	7.74e+10	2.82e-09
250.00	1.16e-20	1.95	1.31e+11	8.31e+10	1.88e-09
260.00	7.86e-21	1.86	1.36e+11	8.87e+10	1.30e-09
270.00	5.48e-21	1.79	1.40e+11	9.41e+10	9.21e-10
280.00	3.94e-21	1.72	1.45e+11	9.94e+10	6.73e-10
290.00	2.90e-21	1.66	1.49e+11	1.05e+11	5.04e-10
298.00	2.30e-21	1.61	1.52e+11	1.09e+11	4.05e-10
300.00	2.18e-21	1.60	1.52e+11	1.10e+11	3.84e-10
310.00	1.67e-21	1.57	1.56e+11	1.14e+11	3.00e-10
320.00	1.31e-21	1.52	1.59e+11	1.19e+11	2.37e-10

S=0.160, 0.320, 0.642, 0.962, 1.604, 2.247, 2.568, 3.209, 3.851, 4.813, at both sides of the IRC

PTS12a

T	Keq	tunn	ktst	kcvt	kt
220.00	1.93e-18	831.17	2.38e+03	2.31e+03	3.70e-12
230.00	9.31e-19	490.02	5.67e+03	5.51e+03	2.51e-12
240.00	4.79e-19	307.38	1.26e+04	1.22e+04	1.80e-12
250.00	2.60e-19	201.57	2.61e+04	2.54e+04	1.33e-12
260.00	1.49e-19	138.76	5.12e+04	4.98e+04	1.03e-12
270.00	8.85e-20	98.92	9.55e+04	9.29e+04	8.14e-13
280.00	5.48e-20	72.89	1.70e+05	1.66e+05	6.64e-13
290.00	3.52e-20	55.28	2.92e+05	2.84e+05	5.52e-13
298.00	2.52e-20	45.07	4.37e+05	4.26e+05	4.84e-13
300.00	2.33e-20	42.86	4.82e+05	4.69e+05	4.68e-13
310.00	1.58e-20	34.09	7.71e+05	7.51e+05	4.05e-13
320.00	1.11e-20	27.76	1.20e+06	1.16e+06	3.56e-13

S= 0.160, 0.320, 0.636, 0.959, 1.599, 2.238, 2.558, 3.198, 3.838, 4.796, at both sides of the IRC

PTS12b

T	Keq	tunn	ktst	kcvt	kt
220.00	1.93e-18	847.95	1.74e+03	1.71e+03	2.79e-12
230.00	9.31e-19	498.79	4.20e+03	4.13e+03	1.92e-12
240.00	4.79e-19	311.42	9.42e+03	9.28e+03	1.38e-12
250.00	2.60e-19	204.10	1.98e+04	1.95e+04	1.04e-12
260.00	1.49e-19	140.05	3.93e+04	3.87e+04	8.05e-13
270.00	8.85e-20	99.86	7.40e+04	7.29e+04	6.45e-13
280.00	5.48e-20	73.66	1.33e+05	1.31e+05	5.29e-13
290.00	3.52e-20	55.51	2.30e+05	2.27e+05	4.43e-13
298.00	2.52e-20	45.32	3.47e+05	3.42e+05	3.91e-13
300.00	2.33e-20	43.12	3.83e+05	3.78e+05	3.79e-13
310.00	1.58e-20	34.32	6.17e+05	6.09e+05	3.31e-13
320.00	1.11e-20	27.87	9.64e+05	9.51e+05	2.93e-13

S= 0.160, 0.320, 0.636, 0.959, 1.599, 2.238, 2.558, 3.198, 3.838, 4.796, at both sides of the IRC

HTS5a

T	Keq	tunn	ktst	kcvt	kt
220.00	1.35e-22	0.99	6.83e+06	1.76e+06	2.35e-16
230.00	1.00e-22	0.96	1.06e+07	2.78e+06	2.67e-16
240.00	7.65e-23	0.93	1.57e+07	4.23e+06	3.01e-16
250.00	5.99e-23	0.91	2.27e+07	6.22e+06	3.38e-16
260.00	4.80e-23	0.89	3.18e+07	8.87e+06	3.78e-16
270.00	3.93e-23	0.87	4.35e+07	1.23e+07	4.20e-16
280.00	3.27e-23	0.86	5.81e+07	1.67e+07	4.68e-16
290.00	2.77e-23	0.85	7.61e+07	2.21e+07	5.21e-16
298.00	2.45e-23	0.84	9.32e+07	2.74e+07	5.64e-16
300.00	2.38e-23	0.84	9.79e+07	2.88e+07	5.76e-16
310.00	2.07e-23	0.83	1.24e+08	3.69e+07	6.35e-16
320.00	1.82e-23	0.82	1.55e+08	4.65e+07	6.98e-16

S=0.173, 0.345, 0.690, 1.035, 1.725, 2.415, 2.761, 3.451, 4.141, 5.176, at both sides of the IRC

HTS6a

T	Keq	tunn	ktst	kcvt	kt
220.00	9.59e-21	637.27	7.16e+06	7.03e+06	4.30e-11
230.00	5.14e-21	379.23	1.33e+07	1.30e+07	2.54e-11
240.00	2.92e-21	237.12	2.34e+07	2.29e+07	1.58e-11
250.00	1.74e-21	154.78	3.94e+07	3.87e+07	1.04e-11
260.00	1.08e-21	105.26	6.39e+07	6.27e+07	7.13e-12
270.00	6.99e-22	74.31	1.00e+08	9.81e+07	5.10e-12
280.00	4.68e-22	54.03	1.52e+08	1.49e+08	3.76e-12
290.00	3.23e-22	40.41	2.25e+08	2.20e+08	2.87e-12
298.00	2.45e-22	32.68	3.01e+08	2.95e+08	2.36e-12
300.00	2.29e-22	31.01	3.24e+08	3.17e+08	2.25e-12
310.00	1.66e-22	24.44	4.56e+08	4.46e+08	1.81e-12
320.00	1.24e-22	19.54	6.29e+08	6.14e+08	1.49e-12

S=0.154, 0.307, 0.614, 0.921, 1.535, 2.150, 2.457, 3.071, 3.686, 4.607, at both sides of the IRC

HTS8a

T	Keq	tunn	ktst	kcvt	kt
220.00	6.94e-20	57803.03	3.41e+00	1.32e+00	5.30e-15
230.00	4.06e-20	27702.70	1.13e+01	4.44e+00	5.00e-15
240.00	2.49e-20	14328.36	3.39e+01	1.34e+01	4.79e-15
250.00	1.60e-20	7882.04	9.33e+01	3.73e+01	4.69e-15
260.00	1.06e-20	4576.80	2.37e+02	9.57e+01	4.65e-15
270.00	7.28e-21	2790.39	5.64e+02	2.29e+02	4.65e-15
280.00	5.15e-21	1776.26	1.26e+03	5.14e+02	4.70e-15
290.00	3.73e-21	1174.31	2.66e+03	1.09e+03	4.78e-15
298.00	2.94e-21	860.10	4.67e+03	1.93e+03	4.88e-15
300.00	2.77e-21	796.38	5.35e+03	2.21e+03	4.88e-15

310.00	2.10e-21	559.72	1.03e+04	4.27e+03	5.03e-15
320.00	1.63e-21	404.04	1.90e+04	7.92e+03	5.21e-15

S=0.156, 0.311, 0.623, 0.935, 1.558, 2.182, 2.493, 3.116, 3.739, at both sides of the IRC

HTS8b

T	Keq	tunn	ktst	kcvt	kt
220.00	6.94e-20	92059.55	1.09e+01	4.03e+00	2.58e-14
230.00	4.06e-20	43281.25	3.40e+01	1.28e+01	2.25e-14
240.00	2.49e-20	22010.87	9.68e+01	3.68e+01	2.02e-14
250.00	1.60e-20	11909.65	2.53e+02	9.74e+01	1.85e-14
260.00	1.06e-20	6820.08	6.16e+02	2.39e+02	1.73e-14
270.00	7.28e-21	4098.36	1.40e+03	5.49e+02	1.64e-14
280.00	5.15e-21	2554.62	3.01e+03	1.19e+03	1.56e-14
290.00	3.73e-21	1663.93	6.14e+03	2.44e+03	1.52e-14
298.00	2.94e-21	1207.64	1.05e+04	4.19e+03	1.49e-14
300.00	2.77e-21	1119.50	1.19e+04	4.77e+03	1.48e-14
310.00	2.10e-21	774.30	2.23e+04	8.95e+03	1.46e-14
320.00	1.63e-21	551.55	3.99e+04	1.61e+04	1.45e-14

S=0.156, 0.311, 0.623, 0.935, 1.558, 2.182, 2.493, 3.116, 3.739, at both sides of the IRC

Reactions starting by HSSCN + OH

BTS1a

T	Keq	ktst	kcvt	kt
220.00	7.58e-21	1.66e+09	1.14e+09	8.64e-12
230.00	5.11e-21	2.14e+09	1.48e+09	7.56e-12
240.00	3.57e-21	2.71e+09	1.87e+09	6.68e-12
250.00	2.58e-21	3.36e+09	2.32e+09	5.99e-12
260.00	1.92e-21	4.09e+09	2.82e+09	5.40e-12
270.00	1.46e-21	4.91e+09	3.38e+09	4.93e-12
280.00	1.14e-21	5.81e+09	4.00e+09	4.54e-12
290.00	9.01e-22	6.80e+09	4.67e+09	4.21e-12
298.00	7.59e-22	7.65e+09	5.24e+09	3.98e-12
300.00	7.29e-22	7.87e+09	5.39e+09	3.93e-12
310.00	5.98e-22	9.01e+09	6.16e+09	3.69e-12
320.00	4.99e-22	1.02e+10	6.98e+09	3.48e-12

S= 0.145, 0.292, 0.592, 0.891, 1.491, 2.090, 2.389, 2.988, 3.586, 4.4667, at both sides of the IRC

Reverse BTS1a

T	Keq	ktst	kt
220.00	2.16e-22	2.08e-02	4.49e-24
230.00	1.72e-22	7.62e-02	1.31e-23
240.00	1.41e-22	2.50e-01	3.52e-23
250.00	1.17e-22	7.47e-01	8.77e-23
260.00	9.96e-23	2.05e+00	2.04e-22

270.00	8.59e-23	5.24e+00	4.50e-22
280.00	7.51e-23	1.25e+01	9.38e-22
290.00	6.64e-23	2.82e+01	1.87e-21
298.00	6.07e-23	5.20e+01	3.16e-21
300.00	5.94e-23	6.03e+01	3.58e-21
310.00	5.36e-23	1.23e+02	6.60e-21
320.00	4.89e-23	2.39e+02	1.17e-20

Conventional TST only

BTS1b

T	Keq	ktst	kcvt	kt
220.00	1.24e-21	2.90e+09	1.90e+09	2.36e-12
230.00	1.00e-21	3.28e+09	2.16e+09	2.16e-12
240.00	8.26e-22	3.66e+09	2.43e+09	2.01e-12
250.00	6.94e-22	4.05e+09	2.71e+09	1.88e-12
260.00	5.94e-22	4.44e+09	2.98e+09	1.77e-12
270.00	5.15e-22	4.83e+09	3.26e+09	1.68e-12
280.00	4.53e-22	5.21e+09	3.54e+09	1.60e-12
290.00	4.03e-22	5.59e+09	3.81e+09	1.54e-12
298.00	3.70e-22	5.89e+09	4.03e+09	1.49e-12
300.00	3.63e-22	5.97e+09	4.08e+09	1.48e-12
310.00	3.29e-22	6.34e+09	4.35e+09	1.43e-12
320.00	3.01e-22	6.70e+09	4.61e+09	1.39e-12

S= 0.473, 0.947, 1.894, 2.841, 3.313, 3.786, 4.731, 5.109, at both sides of the IRC

Reverse BTS1b

T	Keq	ktst	kt
220.00	2.16e-22	6.18e-03	1.33e-24
230.00	1.72e-22	2.36e-02	4.07e-24
240.00	1.41e-22	8.10e-02	1.14e-23
250.00	1.17e-22	2.51e-01	2.95e-23
260.00	9.96e-23	7.16e-01	7.13e-23
270.00	8.59e-23	1.89e+00	1.62e-22
280.00	7.51e-23	4.66e+00	3.50e-22
290.00	6.64e-23	1.08e+01	7.17e-22
298.00	6.07e-23	2.03e+01	1.23e-21
300.00	5.94e-23	2.37e+01	1.41e-21
310.00	5.36e-23	4.94e+01	2.65e-21
320.00	4.89e-23	9.84e+01	4.81e-21

Conventional TST only

BTS2a

T	Keq	ktst	kcvt	kt
220.00	9.67e-21	2.42e+07	1.94e+07	1.88e-13
230.00	6.48e-21	3.56e+07	2.87e+07	1.86e-13
240.00	4.50e-21	5.07e+07	4.09e+07	1.84e-13
250.00	3.22e-21	7.02e+07	5.68e+07	1.83e-13
260.00	2.37e-21	9.49e+07	7.68e+07	1.82e-13
270.00	1.79e-21	1.25e+08	1.02e+08	1.83e-13

280.00	1.39e-21	1.62e+08	1.32e+08	1.83e-13
290.00	1.09e-21	2.07e+08	1.68e+08	1.83e-13
298.00	9.13e-22	2.48e+08	2.01e+08	1.84e-13
300.00	8.75e-22	2.59e+08	2.10e+08	1.84e-13
310.00	7.13e-22	3.20e+08	2.60e+08	1.85e-13
320.00	5.90e-22	3.89e+08	3.17e+08	1.87e-13

S=0.307, 0.614, 1.229, 1.844, 3.073, 4.302, 4.916, -0.307, -0.614, -1.229, -1.844, -3.073, -4.302, -4.916, -6.1467, -7.374, -9.217

Reverse BTS2a

T	Keq	ktst	kt
220.00	4.23e-22	1.46e+00	6.17e-22
230.00	3.39e-22	4.23e+00	1.43e-21
240.00	2.77e-22	1.12e+01	3.11e-21
250.00	2.32e-22	2.74e+01	6.35e-21
260.00	1.97e-22	6.25e+01	1.23e-20
270.00	1.70e-22	1.34e+02	2.28e-20
280.00	1.49e-22	2.73e+02	4.07e-20
290.00	1.32e-22	5.28e+02	6.97e-20
298.00	1.21e-22	8.68e+02	1.05e-19
300.00	1.18e-22	9.78e+02	1.16e-19
310.00	1.07e-22	1.74e+03	1.86e-19
320.00	9.75e-23	2.99e+03	2.91e-19

Conventional TST only

BTS2b

T	Keq	ktst	kcvt	kt
220.00	9.17e-21	1.70e+06	1.57e+06	1.44e-14
230.00	6.15e-21	2.87e+06	2.65e+06	1.63e-14
240.00	4.27e-21	4.63e+06	4.26e+06	1.82e-14
250.00	3.06e-21	7.18e+06	6.62e+06	2.03e-14
260.00	2.26e-21	1.08e+07	9.93e+06	2.24e-14
270.00	1.71e-21	1.57e+07	1.45e+07	2.47e-14
280.00	1.32e-21	2.23e+07	2.05e+07	2.70e-14
290.00	1.04e-21	3.09e+07	2.84e+07	2.95e-14
298.00	8.69e-22	3.95e+07	3.63e+07	3.16e-14
300.00	8.33e-22	4.19e+07	3.85e+07	3.21e-14
310.00	6.79e-22	5.57e+07	5.12e+07	3.48e-14
320.00	5.62e-22	7.28e+07	6.68e+07	3.75e-14

S= 0. 148, 0.298, 0.598, 0.898, 1.498, 2.097, 2.397, 2.997, 3.597, 4.496, at both sides of the IRC

Reverse BTS2b

T	Keq	ktst	kt
220.00	4.23e-22	9.12e-02	3.86e-23
230.00	3.39e-22	3.02e-01	1.02e-22
240.00	2.77e-22	9.06e-01	2.51e-22
250.00	2.32e-22	2.49e+00	5.77e-22
260.00	1.97e-22	6.32e+00	1.25e-21

270.00	1.70e-22	1.50e+01	2.55e-21
280.00	1.49e-22	3.34e+01	4.97e-21
290.00	1.32e-22	7.05e+01	9.30e-21
298.00	1.21e-22	1.23e+02	1.48e-20
300.00	1.18e-22	1.41e+02	1.67e-20
310.00	1.07e-22	2.71e+02	2.90e-20
320.00	9.75e-23	5.00e+02	4.87e-20

Conventional TST only

HTS3a

T	Keq	tunn	ktst	kcvt	kt
220.00	7.58e-21	0.71	2.87e+10	2.41e+10	1.29e-10
230.00	5.11e-21	0.70	3.45e+10	2.89e+10	1.03e-10
240.00	3.57e-21	0.69	4.08e+10	3.41e+10	8.36e-11
250.00	2.58e-21	0.68	4.76e+10	3.96e+10	6.97e-11
260.00	1.92e-21	0.68	5.48e+10	4.55e+10	5.90e-11
270.00	1.46e-21	0.67	6.24e+10	5.16e+10	5.06e-11
280.00	1.14e-21	0.67	7.05e+10	5.81e+10	4.42e-11
290.00	9.01e-22	0.67	7.88e+10	6.47e+10	3.89e-11
298.00	7.59e-22	0.67	8.58e+10	7.02e+10	3.55e-11
300.00	7.29e-22	0.66	8.75e+10	7.16e+10	3.47e-11
310.00	5.98e-22	0.66	9.65e+10	7.87e+10	3.12e-11
320.00	4.99e-22	0.66	1.06e+11	8.59e+10	2.83e-11

S=0.187, 0.374, 0.749, 1.121, 1.8709, 2.619, 2.992, 3.740, 4.485, 5.341, at both sides of the IRC

HTS3b

T	Keq	tunn	ktst	kcvt	kt
220.00	7.58e-21	3.01	4.47e+09	3.42e+09	7.81e-11
230.00	5.11e-21	2.76	5.84e+09	4.46e+09	6.29e-11
240.00	3.57e-21	2.54	7.47e+09	5.70e+09	5.18e-11
250.00	2.58e-21	2.36	9.36e+09	7.12e+09	4.34e-11
260.00	1.92e-21	2.22	1.15e+10	8.75e+09	3.72e-11
270.00	1.46e-21	2.08	1.40e+10	1.06e+10	3.22e-11
280.00	1.14e-21	1.98	1.67e+10	1.26e+10	2.83e-11
290.00	9.01e-22	1.89	1.97e+10	1.48e+10	2.51e-11
298.00	7.59e-22	1.81	2.23e+10	1.67e+10	2.30e-11
300.00	7.29e-22	1.80	2.30e+10	1.72e+10	2.26e-11
310.00	5.98e-22	1.72	2.65e+10	1.99e+10	2.05e-11
320.00	4.99e-22	1.65	3.03e+10	2.27e+10	1.87e-11

S=0.187, 0.374, 0.749, 1.121, 1.8709, 2.619, 2.992, 3.740, 4.485, 5.341, at both sides of the IRC

HTS5a

T	Keq	tunn	ktst	kcvt	kt
220.00	5.92e-18	0.52	5.35e+06	3.93e+06	1.21e-11
230.00	2.56e-18	0.53	9.69e+06	7.15e+06	9.64e-12
240.00	1.19e-18	0.53	1.67e+07	1.24e+07	7.86e-12
250.00	5.89e-19	0.54	2.76e+07	2.05e+07	6.54e-12

260.00	3.09e-19	0.55	4.39e+07	3.27e+07	5.53e-12
270.00	1.70e-19	0.55	6.74e+07	5.05e+07	4.75e-12
280.00	9.82e-20	0.56	1.01e+08	7.54e+07	4.15e-12
290.00	5.90e-20	0.57	1.46e+08	1.10e+08	3.67e-12
298.00	4.03e-20	0.57	1.93e+08	1.46e+08	3.34e-12
300.00	3.67e-20	0.57	2.07e+08	1.56e+08	3.27e-12
310.00	2.36e-20	0.58	2.86e+08	2.16e+08	2.95e-12
320.00	1.56e-20	0.59	3.89e+08	2.94e+08	2.69e-12

S=0.160, 0.319, 0.639, 0.958, 1.596, 2.235, 3.193, 3.832, 4.566, -0.160, -0.319, -0.639, -0.958, -1.596, -2.235, -3.193

HTS6a

T	Keq	tunn	ktst	kcvt	kt
220.00	5.92e-18	11.31	4.37e+03	2.89e+03	1.93e-13
230.00	2.56e-18	9.19	1.13e+04	7.57e+03	1.78e-13
240.00	1.19e-18	7.66	2.72e+04	1.84e+04	1.68e-13
250.00	5.89e-19	6.55	6.08e+04	4.15e+04	1.60e-13
260.00	3.09e-19	5.70	1.28e+05	8.82e+04	1.55e-13
270.00	1.70e-19	5.03	2.56e+05	1.78e+05	1.52e-13
280.00	9.82e-20	4.52	4.88e+05	3.41e+05	1.51e-13
290.00	5.90e-20	4.10	8.89e+05	6.25e+05	1.51e-13
298.00	4.03e-20	3.81	1.40e+06	9.87e+05	1.51e-13
300.00	3.67e-20	3.75	1.56e+06	1.10e+06	1.52e-13
310.00	2.36e-20	3.45	2.64e+06	1.88e+06	1.53e-13
320.00	1.56e-20	3.22	4.33e+06	3.09e+06	1.56e-13

S=0.153, 0.306, 0.610, 0.915, 1.525, 2.136, 2.441, 3.051, 3.661, 4.362, at both sides of the IRC

HTS8a

T	Keq	tunn	ktst	kcvt	kt
220.00	1.53e-19	260734.46	7.19e-01	3.54e-01	1.41e-14
230.00	9.08e-20	115833.33	2.42e+00	1.20e+00	1.26e-14
240.00	5.65e-20	55585.83	7.34e+00	3.67e+00	1.15e-14
250.00	3.66e-20	28543.69	2.04e+01	1.03e+01	1.08e-14
260.00	2.46e-20	15639.10	5.25e+01	2.66e+01	1.02e-14
270.00	1.71e-20	8987.54	1.26e+02	6.42e+01	9.85e-15
280.00	1.22e-20	5434.48	2.83e+02	1.45e+02	9.61e-15
290.00	8.94e-21	3408.36	6.04e+02	3.11e+02	9.48e-15
298.00	7.09e-21	2409.42	1.07e+03	5.52e+02	9.43e-15
300.00	6.71e-21	2208.20	1.22e+03	6.34e+02	9.39e-15
310.00	5.13e-21	1487.80	2.37e+03	1.23e+03	9.40e-15
320.00	4.01e-21	1026.09	4.41e+03	2.30e+03	9.45e-15

S= 0.155, 0.310, 0.620, 0.930, 1.550, 2.170, 2.480, 3.100, 3.720, 4.216 , at both sides of the IRC

HTS8b

T	Keq	tunn	ktst	kcvt	kt
220.00	1.53e-19	301587.30	1.37e+00	6.93e-01	3.20e-14
230.00	9.08e-20	132894.74	4.48e+00	2.28e+00	2.75e-14

240.00	5.65e-20	63475.70	1.32e+01	6.79e+00	2.43e-14
250.00	3.66e-20	32540.54	3.59e+01	1.85e+01	2.20e-14
260.00	2.46e-20	17633.26	9.01e+01	4.69e+01	2.03e-14
270.00	1.71e-20	10090.09	2.11e+02	1.11e+02	1.91e-14
280.00	1.22e-20	6056.91	4.67e+02	2.46e+02	1.82e-14
290.00	8.94e-21	3779.07	9.77e+02	5.16e+02	1.74e-14
298.00	7.09e-21	2671.84	1.70e+03	9.02e+02	1.71e-14
300.00	6.71e-21	2456.31	1.95e+03	1.03e+03	1.70e-14
310.00	5.13e-21	1636.36	3.71e+03	1.98e+03	1.66e-14
320.00	4.01e-21	1129.48	6.79e+03	3.63e+03	1.64e-14

S= 0.155, 0.310, 0.620, 0.930, 1.550, 2.170, 2.480, 3.100, 3.720, 4.216 , at both sides of the IRC

Reactions starting by HSSNO₂ + OH

BTS1a

T	Keq	ktst	kcvt	kt
220.00	7.02e-21	1.32e+09	1.05e+09	7.37e-12
230.00	4.83e-21	1.70e+09	1.35e+09	6.52e-12
240.00	3.44e-21	2.13e+09	1.69e+09	5.81e-12
250.00	2.52e-21	2.61e+09	2.07e+09	5.22e-12
260.00	1.90e-21	3.16e+09	2.51e+09	4.77e-12
270.00	1.47e-21	3.77e+09	2.98e+09	4.37e-12
280.00	1.15e-21	4.43e+09	3.50e+09	4.04e-12
290.00	9.27e-22	5.15e+09	4.07e+09	3.77e-12
298.00	7.88e-22	5.77e+09	4.55e+09	3.58e-12
300.00	7.58e-22	5.92e+09	4.67e+09	3.54e-12
310.00	6.28e-22	6.75e+09	5.31e+09	3.34e-12
320.00	5.28e-22	7.62e+09	5.99e+09	3.17e-12

S= 0.149, 0.299, 0.599, 0.899, 1.499, 2.098, 2.398, 2.998, 3.597, 4.489, at both sides of the IRC

Reverse BTS1a

T	Keq	ktst	kt
220.00	4.39e-19	7.91e+02	3.47e-16
230.00	1.87e-19	2.10e+03	3.94e-16
240.00	8.63e-20	5.16e+03	4.45e-16
250.00	4.24e-20	1.18e+04	5.00e-16
260.00	2.21e-20	2.54e+04	5.60e-16
270.00	1.21e-20	5.17e+04	6.25e-16
280.00	6.93e-21	1.00e+05	6.93e-16
290.00	4.14e-21	1.86e+05	7.70e-16
298.00	2.81e-21	2.96e+05	8.33e-16
300.00	2.56e-21	3.31e+05	8.49e-16
310.00	1.64e-21	5.69e+05	9.35e-16
320.00	1.08e-21	9.46e+05	1.03e-15

Conventional TST only

BTS1b

T	Keq	ktst	kcvt	kt
220.00	4.31e-22	1.02e+09	8.72e+08	3.75e-13
230.00	3.75e-22	1.19e+09	1.02e+09	3.83e-13
240.00	3.32e-22	1.37e+09	1.18e+09	3.92e-13
250.00	2.98e-22	1.55e+09	1.34e+09	3.99e-13
260.00	2.70e-22	1.74e+09	1.50e+09	4.06e-13
270.00	2.48e-22	1.93e+09	1.67e+09	4.14e-13
280.00	2.30e-22	2.13e+09	1.85e+09	4.25e-13
290.00	2.15e-22	2.33e+09	2.02e+09	4.34e-13
298.00	2.04e-22	2.49e+09	2.16e+09	4.41e-13
300.00	2.02e-22	2.53e+09	2.20e+09	4.44e-13
310.00	1.91e-22	2.73e+09	2.38e+09	4.55e-13
320.00	1.82e-22	2.94e+09	2.55e+09	4.64e-13

S= 0.149, 0.299, 0.599, 0.899, 1.499, 2.098, 2.398, 2.998, 3.597, 4.496, at both sides of the IRC

Reverse BTS1b

T	Keq	ktst	kt
220.00	2.59e-22	6.48e+04	1.68e-17
230.00	1.56e-22	1.41e+05	2.19e-17
240.00	9.79e-23	2.89e+05	2.83e-17
250.00	6.41e-23	5.59e+05	3.59e-17
260.00	4.36e-23	1.03e+06	4.49e-17
270.00	3.06e-23	1.81e+06	5.54e-17
280.00	2.21e-23	3.07e+06	6.78e-17
290.00	1.64e-23	5.01e+06	8.21e-17
298.00	1.31e-23	7.25e+06	9.50e-17
300.00	1.24e-23	7.93e+06	9.85e-17
310.00	9.61e-24	1.22e+07	1.17e-16
320.00	7.58e-24	1.82e+07	1.38e-16

Conventional TST only

BTS2a

T	Keq	ktst	kcvt	kt
220.00	4.96e-23	9.20e+07	9.20e+07	4.57e-15
230.00	4.37e-23	1.31e+08	1.31e+08	5.73e-15
240.00	3.90e-23	1.81e+08	1.81e+08	7.06e-15
250.00	3.53e-23	2.44e+08	2.44e+08	8.61e-15
260.00	3.22e-23	3.21e+08	3.21e+08	1.03e-14
270.00	2.97e-23	4.14e+08	4.14e+08	1.23e-14
280.00	2.76e-23	5.25e+08	5.25e+08	1.45e-14
290.00	2.59e-23	6.54e+08	6.54e+08	1.69e-14
298.00	2.47e-23	7.71e+08	7.71e+08	1.90e-14
300.00	2.44e-23	8.03e+08	8.03e+08	1.96e-14
310.00	2.31e-23	9.73e+08	9.73e+08	2.25e-14
320.00	2.21e-23	1.16e+09	1.16e+09	2.56e-14

S= 0.149, 0.299, 0.599, 0.899, 1.499, 2.098, 2.398, 2.998, 3.597, 4.496, at both sides of the IRC

Reverse BTS2a

T	Keq	ktst	kt
220.00	1.22e-23	1.40e-02	1.71e-25
230.00	1.19e-23	4.95e-02	5.90e-25
240.00	1.17e-23	1.58e-01	1.85e-24
250.00	1.15e-23	4.58e-01	5.27e-24
260.00	1.14e-23	1.23e+00	1.40e-23
270.00	1.13e-23	3.05e+00	3.45e-23
280.00	1.13e-23	7.12e+00	8.04e-23
290.00	1.13e-23	1.57e+01	1.77e-22
298.00	1.13e-23	2.84e+01	3.22e-22
300.00	1.13e-23	3.27e+01	3.71e-22
310.00	1.14e-23	6.52e+01	7.43e-22
320.00	1.15e-23	1.24e+02	1.42e-21

Conventional TST only

BTS2b

T	Keq	ktst	kcvt	kt
220.00	4.70e-23	8.31e+08	7.80e+08	3.67e-14
230.00	4.14e-23	1.06e+09	9.90e+08	4.10e-14
240.00	3.70e-23	1.32e+09	1.23e+09	4.55e-14
250.00	3.35e-23	1.61e+09	1.50e+09	5.03e-14
260.00	3.06e-23	1.93e+09	1.80e+09	5.52e-14
270.00	2.83e-23	2.29e+09	2.14e+09	6.06e-14
280.00	2.64e-23	2.68e+09	2.50e+09	6.59e-14
290.00	2.48e-23	3.10e+09	2.89e+09	7.16e-14
298.00	2.37e-23	3.46e+09	3.22e+09	7.62e-14
300.00	2.34e-23	3.56e+09	3.30e+09	7.72e-14
310.00	2.22e-23	4.04e+09	3.75e+09	8.34e-14
320.00	2.13e-23	4.54e+09	4.21e+09	8.95e-14

S= 0.149, 0.299, 0.599, 0.899, 1.499, 2.098, 2.398, 2.998, 3.597, 4.496, at both sides of the IRC

Reverse BTS2b

T	Keq	k2	kt
220.00	1.22e-23	8.08e-02	9.89e-25
230.00	1.19e-23	2.58e-01	3.07e-24
240.00	1.17e-23	7.47e-01	8.72e-24
250.00	1.15e-23	1.99e+00	2.29e-23
260.00	1.14e-23	4.91e+00	5.59e-23
270.00	1.13e-23	1.13e+01	1.28e-22
280.00	1.13e-23	2.47e+01	2.79e-22
290.00	1.13e-23	5.09e+01	5.75e-22
298.00	1.13e-23	8.76e+01	9.92e-22
300.00	1.13e-23	9.99e+01	1.13e-21
310.00	1.14e-23	1.88e+02	2.14e-21
320.00	1.15e-23	3.40e+02	3.90e-21

Conventional TST only

HTS3a

T	Keq	tunn	ktst	kcvt	kt
220.00	7.02e-21	0.27	7.97e+11	3.18e+11	5.95e-10
230.00	4.83e-21	0.26	8.08e+11	3.25e+11	4.10e-10
240.00	3.44e-21	0.26	8.19e+11	3.32e+11	2.92e-10
250.00	2.52e-21	0.25	8.28e+11	3.38e+11	2.14e-10
260.00	1.90e-21	0.25	8.36e+11	3.44e+11	1.62e-10
270.00	1.47e-21	0.24	8.44e+11	3.49e+11	1.25e-10
280.00	1.15e-21	0.24	8.50e+11	3.53e+11	9.84e-11
290.00	9.27e-22	0.24	8.56e+11	3.57e+11	7.89e-11
298.00	7.88e-22	0.24	8.61e+11	3.60e+11	6.70e-11
300.00	7.58e-22	0.24	8.62e+11	3.60e+11	6.45e-11
310.00	6.28e-22	0.23	8.66e+11	3.63e+11	5.35e-11
320.00	5.28e-22	0.23	8.71e+11	3.66e+11	4.49e-11

S=0.164, 0.329, 0.657, 0.985, 1.642, 2.300, 2.628, 3.284, 3.941, 4.925, at both sides of the IRC

HTS3b

T	Keq	tunn	ktst	kcvt	kt
220.00	7.02e-21	1.44	9.49e+09	6.59e+09	6.68e-11
230.00	4.83e-21	1.39	1.19e+10	8.65e+09	5.79e-11
240.00	3.44e-21	1.34	1.47e+10	1.11e+10	5.12e-11
250.00	2.52e-21	1.30	1.78e+10	1.40e+10	4.59e-11
260.00	1.90e-21	1.27	2.12e+10	1.73e+10	4.16e-11
270.00	1.47e-21	0.59	2.50e+10	2.04e+10	1.77e-11
280.00	1.15e-21	0.59	2.91e+10	2.37e+10	1.63e-11
290.00	9.27e-22	0.60	3.35e+10	2.72e+10	1.50e-11
298.00	7.88e-22	0.60	3.73e+10	3.01e+10	1.42e-11
300.00	7.58e-22	0.60	3.82e+10	3.09e+10	1.39e-11
310.00	6.28e-22	0.60	4.32e+10	3.48e+10	1.31e-11
320.00	5.28e-22	0.60	4.85e+10	3.89e+10	1.23e-11

S=0.214, 0.428, 0.956, 1.283, 2.141, 2.997, 3.425, 4.279, 5.129, 6.451, -0.214, -0.428, -0.956, -1.283, -2.141, -2.997, -3.425, -4.282, -5.136, -5.734

FTS10a

T	Keq	ktst	kcvt	kt
220.00	4.16e-23	4.50e+09	4.43e+09	1.84e-13
230.00	3.67e-23	5.37e+09	5.29e+09	1.94e-13
240.00	3.28e-23	6.31e+09	6.21e+09	2.04e-13
250.00	2.97e-23	7.30e+09	7.20e+09	2.14e-13
260.00	2.72e-23	8.36e+09	8.24e+09	2.24e-13
270.00	2.51e-23	9.47e+09	9.33e+09	2.34e-13
280.00	2.34e-23	1.06e+10	1.05e+10	2.46e-13
290.00	2.20e-23	1.18e+10	1.16e+10	2.55e-13
298.00	2.10e-23	1.28e+10	1.26e+10	2.64e-13
300.00	2.08e-23	1.30e+10	1.28e+10	2.66e-13
310.00	1.97e-23	1.43e+10	1.41e+10	2.78e-13

320.00	1.89e-23	1.56e+10	1.53e+10	2.89e-13
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S=0.148, 0.299, v0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.599, 4.499, at both sides of the IRC

FTS10b

T	Keq	ktst	kcvt	kt
220.00	6.01e-21	8.55e+06	7.98e+06	4.79e-14
230.00	4.57e-21	1.24e+07	1.16e+07	5.30e-14
240.00	3.57e-21	1.75e+07	1.63e+07	5.83e-14
250.00	2.86e-21	2.40e+07	2.23e+07	6.38e-14
260.00	2.33e-21	3.20e+07	2.97e+07	6.93e-14
270.00	1.94e-21	4.17e+07	3.87e+07	7.51e-14
280.00	1.64e-21	5.34e+07	4.95e+07	8.12e-14
290.00	1.41e-21	6.71e+07	6.22e+07	8.74e-14
298.00	1.25e-21	7.97e+07	7.37e+07	9.24e-14
300.00	1.22e-21	8.31e+07	7.68e+07	9.37e-14
310.00	1.07e-21	1.01e+08	9.35e+07	1.00e-13
320.00	9.51e-22	1.22e+08	1.12e+08	1.07e-13

S= S=0.148, 0.299, v0.599, 0.899, 1.499, 2.099, 2.399, 2.999, 3.599, 4.499, at both sides of the IRC

HTS5a

T	Keq	tunn	ktst	kcvt	kt
220.00	7.08e-22	5755.29	6.62e+04	6.62e+04	2.70e-13
230.00	5.05e-22	3206.61	1.21e+05	1.21e+05	1.96e-13
240.00	3.73e-22	1885.71	2.10e+05	2.10e+05	1.48e-13
250.00	2.83e-22	1163.32	3.49e+05	3.49e+05	1.15e-13
260.00	2.20e-22	746.86	5.58e+05	5.57e+05	9.16e-14
270.00	1.75e-22	497.09	8.60e+05	8.59e+05	7.49e-14
280.00	1.42e-22	343.75	1.29e+06	1.28e+06	6.26e-14
290.00	1.18e-22	242.78	1.87e+06	1.87e+06	5.34e-14
298.00	1.02e-22	188.66	2.48e+06	2.47e+06	4.76e-14
300.00	9.88e-23	176.98	2.65e+06	2.65e+06	4.63e-14
310.00	8.41e-23	132.15	3.67e+06	3.67e+06	4.08e-14
320.00	7.26e-23	101.00	4.99e+06	4.98e+06	3.65e-14

S= 0.269, 0.539, 1.078, 1.616, 2.6896, 3.776, 4.315, 5.394, 6.470, 7.224 at both sides of the IRC

HTS6a

T	Keq	tunn	ktst	kcvt	kt
220.00	2.07e-21	1.22	9.22e+05	7.46e+05	1.89e-15
230.00	1.19e-21	1.14	1.86e+06	1.51e+06	2.04e-15
240.00	7.15e-22	1.09	3.54e+06	2.87e+06	2.23e-15
250.00	4.50e-22	1.04	6.41e+06	5.20e+06	2.44e-15
260.00	2.95e-22	1.00	1.11e+07	9.02e+06	2.66e-15
270.00	2.00e-22	0.97	1.85e+07	1.50e+07	2.92e-15
280.00	1.40e-22	0.95	2.96e+07	2.41e+07	3.19e-15
290.00	1.01e-22	0.93	4.61e+07	3.75e+07	3.49e-15
298.00	7.86e-23	0.91	6.43e+07	5.22e+07	3.74e-15

300.00	7.41e-23	0.91	6.96e+07	5.66e+07	3.81e-15
310.00	5.59e-23	0.89	1.02e+08	8.33e+07	4.16e-15
320.00	4.30e-23	0.88	1.47e+08	1.20e+08	4.55e-15

S=0.153, 0.307, 0.613, 0.920, 1.288, -0.153, -0.306, -0.614, -0.920, -1.533, -2.145, -2.452, -3.065, -3.678, -4.107

HTS8a

T	Keq	tunn	ktst	kcvt	kt
220.00	5.16e-19	781501.34	1.93e+01	7.46e+00	3.01e-12
230.00	2.92e-19	332300.88	5.77e+01	2.26e+01	2.19e-12
240.00	1.73e-19	153035.14	1.57e+02	6.26e+01	1.66e-12
250.00	1.08e-19	75625.00	3.96e+02	1.60e+02	1.31e-12
260.00	6.98e-20	39841.69	9.29e+02	3.79e+02	1.05e-12
270.00	4.67e-20	22301.30	2.05e+03	8.43e+02	8.79e-13
280.00	3.23e-20	12994.35	4.26e+03	1.77e+03	7.43e-13
290.00	2.30e-20	7909.60	8.44e+03	3.54e+03	6.43e-13
298.00	1.78e-20	5469.80	1.41e+04	5.96e+03	5.80e-13
300.00	1.67e-20	5000.00	1.60e+04	6.76e+03	5.66e-13
310.00	1.25e-20	3274.19	2.90e+04	1.24e+04	5.07e-13
320.00	9.49e-21	2211.01	5.08e+04	2.18e+04	4.58e-13

S= 0.1545, 0.309, 0.618, 0.928, 1.547, 2.167, 2.475, 3.095, 3.713, 4.147, at both sides of the IRC

HTS8b

T	Keq	tunn	ktst	kcvt	kt
220.00	5.16e-19	871212.12	5.51e+01	2.64e+01	1.19e-11
230.00	2.92e-19	368906.46	1.56e+02	7.59e+01	8.17e-12
240.00	1.73e-19	170351.76	4.05e+02	1.99e+02	5.88e-12
250.00	1.08e-19	84123.71	9.76e+02	4.85e+02	4.40e-12
260.00	6.98e-20	44272.73	2.20e+03	1.10e+03	3.40e-12
270.00	4.67e-20	24491.53	4.66e+03	2.36e+03	2.70e-12
280.00	3.23e-20	14246.86	9.36e+03	4.78e+03	2.20e-12
290.00	2.30e-20	8645.72	1.79e+04	9.23e+03	1.83e-12
298.00	1.78e-20	5980.13	2.92e+04	1.51e+04	1.61e-12
300.00	1.67e-20	5438.60	3.29e+04	1.71e+04	1.56e-12
310.00	1.25e-20	3564.36	5.81e+04	3.03e+04	1.35e-12
320.00	9.49e-21	2384.62	9.91e+04	5.20e+04	1.18e-12

S= 0.1545, 0.309, 0.618, 0.928, 1.547, 2.167, 2.475, 3.095, 3.713, 4.147, at both sides of the IRC

Table S7. RMS and MAE of the difference in the relative energies computed at CCSD(T)/aug-cc-pV(T+d)Z level of theory over optimized geometries obtained at BH&HLYP/6-311+G(2df,2p) and QCISD/6-311+G(2df,2p) levels of theory.

Reaction	RMS	MAE
HSSH + OH	0.39	-1.34
HSSCH₃ + OH	0.56	-1.27
HSSNH₂ + OH	0.55	1.44

HSSCOOH + OH	0.36	-1.18
HSSCN + OH	0.37	-1.09
HSSNO² + OH	0.62	-1.58

Table S8. Cartesian coordinates (in Angstrom) of all stationary points investigated.

Reactions starting by HSSH + OH

BH&HLYP/6-311+G(2df,2p) optimized geometries

HSSH

```
H -0.060670 -0.054583 -0.007322
S 0.026007 0.048606 1.319357
S 2.079107 0.004448 1.494867
H 2.311543 1.315414 1.419415
```

OH

```
8 0.000000 0.000000 0.004208
1 0.000000 0.000000 0.965792
```

CRFTS1a = CRBTS1b = CRPTS3a = CRHTS3a

```
H -0.926892 1.249114 0.003981
S -1.368739 -0.009588 0.005474
S 0.476466 -0.919605 -0.067204
H 0.750405 -0.941530 1.237400
O 1.538535 1.576696 0.125888
H 2.082202 1.409436 -0.64682
```

FTS1a

```
H -1.106328 1.350168 0.282399
S -1.378202 0.077931 -0.002865
S 0.678379 -0.696456 -0.071295
H 1.026832 -0.895238 1.203289
O 1.165050 1.041624 0.037389
H 2.034550 1.067216 -0.355787
```

CPFTS1a = CPFTS1b

```
H -1.262804 1.268774 0.215461
S -1.985646 0.148778 0.255842
S 1.068090 -0.691113 -0.127757
H 1.117592 -1.015736 1.167914
O 1.401710 0.916004 0.009179
H 2.338397 1.050928 -0.090079
```

CRFTS1b = CRBTS1a = CRHTS3b

```
H 2.168206 -0.957701 0.082441
S 1.367456 0.101991 -0.040800
S -0.424510 -0.912216 -0.109436
H -0.750755 -0.834047 1.180385
O -1.712967 1.524546 0.199409
H -1.994592 1.434971 -0.713741
```

FTS1b

```
H 1.949930 -0.914608 -0.043751
S 1.295660 0.245670 0.008978
S -0.640732 -0.720682 -0.075202
H -1.044116 -0.917443 1.184632
O -1.202826 1.011629 0.080388
H -1.940310 1.078178 -0.521150
```

BTS1a

```
S -0.092883 0.100499 0.026367
S -0.246953 0.411448 2.103269
```


H	1.210742	-0.138156	0.017332
H	-1.056935	-0.621450	2.335787
O	0.368053	1.032927	-1.817421
H	-0.439897	1.503084	-2.019613

CPBTS1a

S	-0.033423	0.187129	-0.136883
S	-0.246916	0.354574	2.193830
H	1.268043	0.155070	0.099034
H	-1.565334	0.183299	2.127708
O	0.282920	0.942806	-1.639678
H	-0.537102	0.994277	-2.122318

BTS1b

S	-0.327946	0.132710	0.064892
S	-0.003384	0.017947	2.129177
H	1.299501	-0.229078	2.088616
O	0.121610	-1.301638	3.812281
H	-0.801812	-1.414838	4.035092
H	-0.277831	-1.172570	-0.203723

CPBTS1b

S	-0.363275	0.158831	-0.025959
S	0.001165	-0.134340	2.289745
H	1.269929	-0.392199	2.018808
O	0.089899	-1.149015	3.659959
H	-0.676126	-0.977426	4.200323
H	0.274032	-0.944896	-0.413388

PTS3a

H	0.473739	0.091043	-0.103333
S	-0.012130	-0.065171	1.288229
S	1.993410	-0.033427	1.623541
H	2.314455	-1.297166	1.332912
O	1.662319	0.138897	-0.842802
H	1.897692	1.027099	-1.109905

HTS3b

H	-0.215484	-0.206801	-0.050182
S	0.118138	0.034895	1.272761
S	2.155325	-0.008018	1.120577
H	2.340891	-1.326663	1.207978
O	-0.634675	0.066143	-1.502124
H	-0.444447	1.003563	-1.588196

CPPTS3a = CPHTS3b

H	-1.450057	0.114338	-1.345892
S	-0.519632	0.008742	1.160903
S	1.213607	-0.307622	0.277157
H	0.840794	-0.229979	-1.009449
O	-1.027678	0.000598	-2.193008
H	-1.421702	0.636238	-2.777386

HTS3a

H	-0.022725	0.037435	0.021795
S	0.037023	0.005178	1.405674
S	2.065675	-0.020921	1.649829
H	2.239728	-1.337731	1.776995
O	-0.264329	-0.451018	-1.415447
H	-0.356434	-1.399787	-1.299854

CPHTS3a

H	-1.131884	-0.166663	-1.613202
S	-0.626336	-0.078547	0.914561
S	1.271358	-0.407059	0.501652
H	1.805832	-0.348983	1.728453
O	-1.014640	-0.215535	-2.557751
H	-1.664411	-0.832808	-2.869484

HS2

S	-0.008073	0.000000	-0.005559
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S	0.006939	0.000000	1.964358
H	1.321995	0.000000	2.219970

CRHTS5a

H	-0.912506	0.811505	-1.417185
S	-1.096127	0.626392	-0.105040
O	0.132204	1.522959	0.475531
H	0.901997	0.951786	0.524287
S	0.858413	-1.463093	-0.225841
H	0.293034	-1.945025	0.880105

HTS5a

H	0.141228	0.279085	-0.074652
S	-0.065524	0.026582	1.228479
O	1.412189	-0.111643	1.736363
H	1.856697	-1.135710	1.604119
S	2.464851	-2.661350	1.460955
H	1.977714	-3.047295	2.640304

CPHTS5a = CPHTS5b

H	-0.878370	0.381304	-1.123628
S	-1.167177	1.574543	-0.546252
O	-0.218040	1.637276	0.604912
H	1.074836	-0.339079	0.576466
S	1.274550	-1.455478	-0.126200
H	0.567793	-2.205401	0.716181

CRHTS5b

H	-0.982519	0.539184	-1.479650
S	-1.056238	0.485406	-0.143968
O	0.151646	1.510822	0.233413
H	0.953089	0.988621	0.311392
S	1.048577	-1.511825	0.085315
H	1.084724	-1.559415	-1.246516

HTS5b

H	-0.176176	0.022558	0.093919
S	0.029328	0.106944	1.418779
O	1.592525	-0.009131	1.477866
H	1.972467	-1.065927	1.529997
S	2.496057	-2.628788	1.588255
H	3.359747	-2.470498	0.585081

CRHTS6a

H	-2.064043	2.055503	-0.438150
O	-1.884036	1.160572	-0.708655
S	-0.468471	0.663087	-0.021224
H	0.342178	0.911823	-1.050857
S	1.131995	-1.655425	0.137622
H	0.535406	-1.899616	1.303684

HTS6a

H	-0.070399	-0.165804	0.075857
O	0.075452	-0.128128	1.016256
S	1.633891	0.242749	1.319141
H	2.225950	-1.114319	1.247849
S	2.769621	-2.712794	1.342308
H	2.216598	-2.835418	2.548976

CPHTS6a = CPHTS6b

H	-1.110484	0.122819	-0.446490
O	-1.627593	0.934498	-0.491065
S	-0.664120	2.206729	-0.286494
H	1.423346	-0.651856	0.058966
S	0.519599	-1.579290	-0.252802
H	0.293016	-1.897245	1.020280

CRHTS6b

H	-1.353911	0.100878	-0.672613
O	-1.213094	1.043157	-0.556623
S	0.239910	1.228582	0.153402

H	-0.123837	1.154306	1.438670
S	0.313039	-1.633344	0.110751
H	1.136468	-1.515331	-0.929968

HTS6b

H	0.010227	-0.052469	-0.020586
O	0.035923	-0.001824	0.929869
S	1.582765	-0.020185	1.442753
H	1.750754	-1.478673	1.646364
S	1.977080	-3.154401	1.580964
H	2.702860	-3.031228	0.469572

HSOH

H	0.029075	-0.041630	0.009640
S	-0.012532	0.033760	1.343827
O	1.610071	0.015669	1.641964
H	1.889386	-0.883676	1.774040

SH2

H	0.002817	0.000000	0.001547
S	0.000127	0.000000	1.332416
H	1.328916	0.000000	1.406229

QCISD/6-311+G(2df,2p) optimized geometries

oh-qci-b2

O	0.000000	0.000000	0.000572
H	0.000000	0.000000	0.969428

hssh-qci-b2

H	-0.058507	-0.054427	-0.011027
S	0.018483	0.050173	1.324005
S	2.086126	-0.001097	1.494854
H	2.309885	1.319235	1.418485

CRFTS1a = CRBTS1b = CRPTS3a = CRHTS3a

H	-0.939663	1.303684	0.146981
S	-1.428454	0.055302	0.097181
S	0.405749	-0.893070	-0.095151
H	0.724298	-0.973296	1.204808
O	1.511250	1.509222	0.257979
H	2.039518	1.381358	-0.542661

FTS1a

H	-1.097626	1.348962	0.294913
S	-1.392699	0.079196	-0.014844
S	0.691184	-0.700661	-0.073217
H	1.025158	-0.898228	1.213642
O	1.156975	1.053700	0.032313
H	2.037287	1.062277	-0.359679

CPFTS1a = CPFTS1b

H	-0.822083	0.897113	-0.053118
S	-2.000166	0.576637	0.511054
S	1.807199	-0.787741	-0.058984
H	0.943518	-0.969169	0.955943
O	1.447191	0.817368	-0.379461
H	2.055448	1.354146	0.132739

CRFTS1b = CRBTS1a = CRHTS3b

H	2.127870	-0.932401	0.051003
S	1.304486	0.118181	-0.083058
S	-0.471764	-0.955756	-0.126812
H	-0.790502	-0.844984	1.170680
O	-1.676722	1.545991	0.239366
H	-2.029043	1.423365	-0.653979

FTS1b

H	1.949446	-0.924054	-0.035533
S	1.308581	0.253643	0.007182

S	-0.645695	-0.718979	-0.084169
H	-1.044403	-0.922496	1.184539
O	-1.193373	1.028333	0.073848
H	-1.956949	1.066297	-0.511971

BTS1a

S	-0.146958	0.056936	0.025581
S	-0.327537	0.474877	2.079824
H	1.166918	-0.178759	0.029761
H	-0.950570	-0.668937	2.400459
O	0.413022	1.064749	-1.862975
H	-0.412748	1.539486	-2.026929

CPBTS1a

S	-0.067482	0.185658	-0.132188
S	-0.327319	0.401626	2.161042
H	1.237987	0.166419	0.126230
H	-1.650356	0.217203	2.057522
O	0.300336	0.918855	-1.668897
H	-0.528969	0.949546	-2.155006

BTS1b

S	-0.268698	0.108120	0.032910
S	0.023471	0.133983	2.101436
H	1.328733	-0.153086	2.104980
O	0.126750	-1.379445	3.826638
H	-0.826798	-1.455052	3.968033
H	-0.373321	-1.221987	-0.107663

CPBTS1b

S	-0.367712	0.164063	-0.015294
S	-0.005941	-0.125348	2.272627
H	1.268221	-0.396073	2.002232
O	0.098302	-1.162471	3.662283
H	-0.680862	-0.971671	4.192768
H	0.283617	-0.947546	-0.385129

HTS3a

H	-0.046359	0.089948	0.037087
S	0.014471	0.017818	1.418049
S	2.065361	-0.031875	1.626737
H	2.212254	-1.361936	1.726403
O	-0.263990	-0.463693	-1.421444
H	-0.282800	-1.417107	-1.247841

CPHTS3a

H	-1.174227	-0.158271	-1.547160
S	-0.691586	-0.041250	0.978340
S	1.174948	-0.420003	0.401440
H	1.802597	-0.362521	1.592293
O	-0.913547	-0.237418	-2.467834
H	-1.558265	-0.830132	-2.852850

HTS3b

H	-0.267496	-0.248995	-0.010837
S	0.085551	0.028351	1.299236
S	2.134573	0.025200	1.068599
H	2.335972	-1.298417	1.160366
O	-0.657257	0.076624	-1.497499
H	-0.311595	0.980356	-1.559049

PTS3a

H	0.465872	0.061832	-0.103172
S	-0.029710	-0.038619	1.293719
S	2.000764	-0.006335	1.592816
H	2.308435	-1.274440	1.274750
O	1.684688	0.098973	-0.833832
H	1.899437	1.019864	-1.035639

CPPTS3a

H	0.900072	0.452510	-0.547755
S	0.100150	0.192147	1.990062
S	1.765495	-0.881735	2.177381
H	2.256216	-0.754718	0.927597
O	1.648453	0.096437	-1.033837
H	1.924351	0.801366	-1.619138

HS2	hs2-qci		
S	-0.008073	0.000000	-0.015382
S	0.002231	0.000000	1.973380
H	1.326703	0.000000	2.220771

Reactions starting by HSSCH₃ + OH

BH&HLYP/6-311+G(2df,2p) optimized geometries

CH3SSH			
H	0.037441	0.099995	0.030864
S	0.011191	-0.051260	1.357326
S	2.028165	-0.002300	1.729170
C	2.358877	1.761495	1.930886
H	3.400946	1.838495	2.214084
H	2.200321	2.294504	1.005619
H	1.743588	2.178187	2.713412

CH3SOH			
C	-0.006264	-0.002036	0.009996
S	0.017365	-0.019174	1.798554
H	1.031529	0.023032	-0.300597
H	-0.472606	-0.889721	-0.393989
H	-0.505651	0.884455	-0.353515
O	-1.599357	0.067333	2.125678
H	-1.944537	-0.813806	2.221986

CH3S			
C	0.002203	0.006491	0.004257
S	-0.001543	-0.006266	1.794578
H	1.007290	-0.003315	-0.389823
H	-0.495911	-0.904597	-0.311708
H	-0.554711	0.845968	-0.384473

CH2SSH			
C	0.002435	0.059806	-0.002756
S	0.017136	0.092883	1.702006
H	0.908909	0.072447	-0.570913
H	-0.957376	0.112356	-0.476758
S	1.857660	-0.689409	2.209212
H	2.522523	0.462982	2.308656

CH3SH			
C	0.000487	-0.001236	0.003951
S	-0.000741	-0.011611	1.814760
H	1.317867	0.014678	1.990969
H	-1.035730	-0.021150	-0.299856
H	0.495532	-0.874180	-0.392636
H	0.458693	0.896063	-0.382255

CH3SO			
C	-0.000282	-0.002796	0.000659
S	0.000900	-0.020179	1.795359
O	1.427509	0.023628	2.203369
H	-1.029950	-0.034470	-0.331232
H	0.474833	0.902569	-0.349937
H	0.534448	-0.867427	-0.366587

CRBTS1a = CRFTS1b

S	-0.549076	0.260301	-0.181576
S	-0.320031	-0.029590	1.838380
H	0.710144	0.563918	-0.500841
C	-0.573300	1.628813	2.507510
O	0.697553	-1.724889	-1.849075
H	-0.053523	-2.257093	-1.576049
H	-0.540642	1.521711	3.584215
H	0.212469	2.298061	2.191624
H	-1.537037	2.016417	2.215308

BTS1a

S	0.065736	-0.044655	-0.061294
S	0.063259	0.025654	2.036105
H	1.381817	-0.109858	-0.200780
C	-0.807890	1.585893	2.308884
O	0.115173	-1.297242	-1.746489
H	-0.786753	-1.607886	-1.806929
H	-0.924242	1.676855	3.380725
H	-0.234558	2.419997	1.935241
H	-1.785879	1.567598	1.852239

CPBTS1a

S	0.277918	-0.169480	-0.105242
S	0.113526	0.049199	2.176686
H	1.169599	-1.113255	0.149906
C	-0.991052	1.472106	2.180653
O	-0.081432	-0.985472	-1.587132
H	-0.679428	-0.435688	-2.084759
H	-0.871472	1.972768	3.131356
H	-0.731870	2.160527	1.387991
H	-2.020373	1.162167	2.079538

CRBTS1b = CRFTS1a = CRHTS3b

S	0.136130	-0.488523	0.121420
S	-0.129346	-0.071346	2.113758
H	1.356482	0.021465	-0.049123
O	-0.177373	1.901981	-1.223323
H	-0.954704	1.493722	-1.610234
C	-0.750161	1.624626	2.103068
H	-0.027235	2.298825	1.672561
H	-1.682644	1.689690	1.564826
H	-0.914044	1.877817	3.142857

BTS1b

S	0.118282	0.011489	-0.025311
S	-0.310839	-0.130348	2.007175
H	1.270906	0.662215	0.079663
O	-0.064570	1.242581	-1.738836
H	-0.935159	1.005439	-2.054753
C	-0.665128	1.583695	2.451460
H	0.210401	2.204000	2.331101
H	-1.480102	1.970088	1.858956
H	-0.953201	1.571097	3.494065

CPBTS1b

S	0.119807	0.176703	-0.183411
S	-0.402242	-0.137967	2.029290
H	0.980014	1.113166	0.184643
O	-0.058516	1.006025	-1.695754
H	-0.518626	0.420671	-2.290325
C	-0.606925	1.559457	2.601152
H	0.272028	2.154198	2.393793
H	-1.472912	2.013132	2.142664
H	-0.760176	1.523197	3.671090

FTS1b

H	-0.009670	-0.031231	0.124358
S	0.049509	-0.124669	1.459383
S	2.113608	0.004854	2.104179

C	2.170162	1.788474	2.343791
O	0.474233	-1.868129	1.244828
H	-0.236837	-2.344258	1.665765
H	3.131423	1.994467	2.796208
H	2.104383	2.320383	1.406175
H	1.392011	2.120623	3.015356

CPFTS1b

H	-0.683546	-0.882178	0.006762
S	-0.742017	-0.380093	1.245112
S	3.130629	0.332651	1.705907
C	2.438870	1.756998	2.541879
O	0.312326	-1.392673	1.991899
H	1.195536	-1.021423	1.917755
H	2.320433	1.498027	3.588005
H	3.077606	2.621508	2.453023
H	1.454746	1.962737	2.142787

FTS1a

H	0.178431	0.214177	0.023654
S	-0.021215	0.018005	1.331656
S	1.968594	-0.062089	2.272407
C	2.698396	1.588581	2.387972
O	-0.002326	1.773105	1.645264
H	-0.924988	2.008417	1.704114
H	3.692520	1.426114	2.787907
H	2.777496	2.050012	1.416909
H	2.129950	2.215685	3.052836

CPFTS1a

H	-0.831263	-0.792756	-0.499966
S	-1.977912	-0.182944	-0.176002
S	1.925843	-0.057498	-0.894715
H	-0.831263	-0.792756	-0.499966
S	-1.977912	-0.182944	-0.176002
S	1.925843	-0.057498	-0.894715
C	1.687375	1.010339	0.522036
O	-1.545837	1.356152	-0.608081
H	-1.794769	1.500402	-1.514480
H	1.505278	0.398199	1.396454
H	2.534316	1.657144	0.689448
H	0.792157	1.595511	0.348423

CBTS2a = CRFTS2b

S	-0.549076	0.260301	-0.181576
S	-0.320031	-0.029590	1.838380
H	0.710144	0.563918	-0.500841
C	-0.573300	1.628813	2.507510
O	0.697553	-1.724889	-1.849075
H	-0.053523	-2.257093	-1.576049
H	-0.540642	1.521711	3.584215
H	0.212469	2.298061	2.191624
H	-1.537037	2.016417	2.215308

BTS2a

S	0.065736	-0.044655	-0.061294
S	0.063259	0.025654	2.036105
H	1.381817	-0.109858	-0.200780
C	-0.807890	1.585893	2.308884
O	0.115173	-1.297242	-1.746489
H	-0.786753	-1.607886	-1.806929
H	-0.924242	1.676855	3.380725
H	-0.234558	2.419997	1.935241
H	-1.785879	1.567598	1.852239

CPBTS2a

S	0.277918	-0.169480	-0.105242
S	0.113526	0.049199	2.176686
H	1.169599	-1.113255	0.149906
C	-0.991052	1.472106	2.180653

O	-0.081432	-0.985472	-1.587132
H	-0.679428	-0.435688	-2.084759
H	-0.871472	1.972768	3.131356
H	-0.731870	2.160527	1.387991
H	-2.020373	1.162167	2.079538

CRBTS2b = CRFTS2a

S	0.136130	-0.488523	0.121420
S	-0.129346	-0.071346	2.113758
H	1.356482	0.021465	-0.049123
O	-0.177373	1.901981	-1.223323
H	-0.954704	1.493722	-1.610234
C	-0.750161	1.624626	2.103068
H	-0.027235	2.298825	1.672561
H	-1.682644	1.689690	1.564826
H	-0.914044	1.877817	3.142857

BTS2b

S	0.118282	0.011489	-0.025311
S	-0.310839	-0.130348	2.007175
H	1.270906	0.662215	0.079663
O	-0.064570	1.242581	-1.738836
H	-0.935159	1.005439	-2.054753
C	-0.665128	1.583695	2.451460
H	0.210401	2.204000	2.331101
H	-1.480102	1.970088	1.858956
H	-0.953201	1.571097	3.494065

CPBTS2b = CPFTS2a

S	0.119807	0.176703	-0.183411
S	-0.402242	-0.137967	2.029290
H	0.980014	1.113166	0.184643
O	-0.058516	1.006025	-1.695754
H	-0.518626	0.420671	-2.290325
C	-0.606925	1.559457	2.601152
H	0.272028	2.154198	2.393793
H	-1.472912	2.013132	2.142664
H	-0.760176	1.523197	3.671090

FTS2b

C	0.132153	0.106998	-0.062428
S	0.159841	0.225706	1.728386
S	1.947726	-0.718775	2.512866
H	2.614728	0.431948	2.612485
O	-0.488584	-1.492861	1.776832
H	-0.977774	-1.547598	2.593448
H	0.787824	-0.698372	-0.354958
H	-0.875427	-0.109722	-0.382687
H	0.481546	1.045153	-0.466853

CPFTS2b

C	0.016601	0.030024	-0.045839
S	-0.168803	0.204661	1.720441
S	2.532154	-0.058643	2.232158
H	2.316381	0.534612	3.404661
O	-0.312984	-1.343509	2.192960
H	0.569480	-1.658478	2.403337
H	-0.848227	-0.472696	-0.453247
H	0.075696	1.034591	-0.445086
H	0.921371	-0.508049	-0.286926

FTS2a

C	0.082151	-0.043306	-0.033122
S	0.251419	-0.163804	1.744408
S	2.291860	0.571070	2.134490
H	2.047005	1.879313	2.191541
O	-0.254369	1.538108	2.138141
H	-1.138611	1.438732	2.482994
H	-0.249423	0.950577	-0.291203
H	1.032163	-0.255536	-0.500357
H	-0.656479	-0.775093	-0.330984

CRPTS3a = CRPTS3b = CRHTS3a

H	-1.760901	0.194505	-0.355333
S	-1.220949	0.281856	0.863203
S	0.735015	0.277526	0.252955
C	1.112060	-1.472858	0.071223
O	0.014635	0.243312	-2.118079
H	0.377371	1.101640	-2.337733
H	2.154412	-1.526854	-0.214504
H	0.963783	-1.985588	1.009034
H	0.502090	-1.898497	-0.709088

PTS3a

H	-0.059710	0.062882	-0.031701
S	-0.075538	0.044423	1.443145
S	1.924462	-0.001508	1.069900
C	2.294940	-1.743768	0.838712
O	0.896847	0.012044	-1.091112
H	1.046686	0.865744	-1.492536
H	3.334333	-1.811611	0.547257
H	2.133835	-2.268872	1.768119
H	1.661958	-2.134900	0.058624

CPPTS3a = CPPTS3b = CPHTS3a = CPHTS3b

H	-0.802693	0.272398	-1.663298
S	-0.869259	0.722310	0.847586
S	0.769559	-0.200193	1.381597
C	1.216139	-1.300164	0.020159
O	-0.421656	-0.010957	-2.491302
H	-0.813009	0.532176	-3.163955
H	2.156794	-1.757885	0.295091
H	0.457504	-2.058753	-0.097539
H	1.320622	-0.740446	-0.895956

PTS3b

H	0.004286	-0.065893	-0.002808
S	0.041878	-0.046227	1.460438
S	2.034461	-0.049761	1.098993
C	2.461965	-1.795299	1.004293
O	0.922250	0.090001	-1.093849
H	1.098508	-0.589076	-1.742956
H	3.491552	-1.855982	0.678003
H	2.358237	-2.244385	1.980785
H	1.814584	-2.290938	0.298077

HTS3a

H	-0.077291	0.046774	0.039952
S	-0.034870	0.123079	1.415829
S	1.976607	0.025558	1.706627
C	2.325926	-1.742063	1.589718
O	-0.139920	0.542646	-1.464706
H	0.117633	1.461885	-1.359363
H	3.378524	-1.855439	1.814896
H	1.741280	-2.292663	2.310370
H	2.131931	-2.104056	0.591542

HTS3b

H	0.026239	0.052558	-0.038925
S	-0.017566	0.118602	1.339274
S	1.971286	0.033435	1.754015
C	2.281469	-1.734569	1.946827
O	-0.121274	-0.589428	-1.476353
H	-0.521715	-1.439275	-1.277879
H	3.312067	-1.825361	2.264835
H	1.634280	-2.155836	2.700599
H	2.150962	-2.248799	1.006618

CRHTS11a = CRHTS1b

S	-0.024515	0.222146	-0.069579
S	0.088497	-0.355936	1.898287
C	1.686800	0.115430	-0.637673

H	2.087596	-0.874095	-0.481927
H	1.652519	0.327101	-1.698728
H	2.303989	0.853761	-0.148396
H	0.421474	0.811132	2.456121
O	3.014516	-2.199443	1.813640
H	2.176602	-1.745603	1.975328

HTS11a

S	-0.008096	-0.027271	0.012157
S	-0.113261	0.021165	2.062852
C	1.731856	-0.024978	-0.298906
H	2.238743	-1.047865	0.105330
H	1.891726	-0.045758	-1.368412
H	2.261643	0.786663	0.173697
H	-0.033099	1.342082	2.239810
O	2.858522	-2.054501	0.654688
H	2.632045	-1.883411	1.569839

CPHTS11a = CPHTS11b

S	-0.073009	-0.105156	0.243906
S	-0.168086	0.598193	2.176001
C	1.508112	0.294189	-0.266357
H	2.810958	-1.578727	0.489019
H	1.784626	-0.050582	-1.244353
H	2.077523	1.049118	0.235726
H	-0.633085	1.818277	1.900352
O	3.406124	-2.310569	0.621757
H	2.918385	-2.952072	1.123199

HTS11b

S	0.096122	-0.169637	0.012842
S	0.064089	-0.051765	2.063286
C	1.804123	0.044234	-0.395298
H	2.461562	-0.926748	-0.1111050
H	1.889352	0.148166	-1.467833
H	2.279219	0.857150	0.131489
H	-0.100550	1.268047	2.175485
O	3.171969	-2.013035	0.091577
H	2.459410	-2.650182	0.029276

CRHTS5a = CRHTS5b

H	-1.046557	1.847047	-1.760004
S	-1.402026	1.456197	-0.531250
O	0.029680	1.675611	0.241408
H	0.543092	0.866741	0.167427
S	1.362168	-1.349222	-0.049290
C	-0.039860	-2.130041	0.744798
H	-0.954683	-1.732941	0.325839
H	-0.007225	-3.203688	0.647440
H	-0.015760	-1.858727	1.794208

HTS5a

H	0.187734	0.084812	-0.216467
S	-0.010584	-0.046585	1.106057
O	1.464801	-0.022528	1.632053
H	2.033889	-1.042668	1.603934
S	2.645126	-2.511915	1.572699
C	1.180605	-3.352441	2.192571
H	0.288615	-2.885889	1.789994
H	1.203797	-4.373192	1.834362
H	1.141802	-3.350985	3.271275

CPHTS5a = CPHTS5b

H	-0.245590	0.881502	-1.407444
S	-1.251555	1.720952	-1.056075
O	-1.569851	1.303483	0.343032
H	1.826080	-0.374832	0.592889
S	1.283412	-1.215268	-0.284743
C	-0.065683	-1.820005	0.764231
H	-0.710019	-1.009232	1.064193
H	-0.628541	-2.516376	0.160098

H 0.323083 -2.341394 1.625070

HTS5b

C -0.089058 0.041379 -0.032641
S -0.029315 -0.160329 1.756480
H 0.836413 -0.263810 -0.497197
H -0.919177 -0.504424 -0.456391
H -0.242286 1.095895 -0.224564
H 0.227966 -1.734222 1.801006
O 0.416537 -2.883618 1.832319
S 1.062623 -3.378572 3.173053
H 2.367005 -3.202235 2.903191

CRHTS6a

H -1.311396 0.846594 -1.897080
O -1.438709 0.725833 -0.962438
S -0.551867 1.866468 -0.153030
H 0.571866 1.154115 -0.005429
S 1.364560 -1.610364 0.007283
C -0.167580 -1.883971 0.891797
H -0.111068 -1.389257 1.853338
H -0.962963 -1.406077 0.332336
H -0.377457 -2.933775 1.024241

HTS6a

H 0.265772 -0.529531 -0.493719
O 0.031033 -0.606240 0.425927
S 1.192052 0.086068 1.346350
H 2.116982 -1.111987 1.462738
S 2.799047 -2.598207 1.567256
C 1.387729 -3.380239 2.367611
H 1.260052 -3.024071 3.378018
H 0.486947 -3.220442 1.794277
H 1.598765 -4.441887 2.391119

CPHTS6a = CPHTS6b

H -0.335708 0.379164 -1.217603
O -0.931827 1.078768 -1.517442
S -1.553145 1.845912 -0.248618
H 1.592137 -0.355952 0.612320
S 0.954362 -1.218482 -0.175932
C -0.254170 -1.812017 1.036327
H 0.240268 -2.330442 1.842683
H -0.850073 -0.997078 1.415340
H -0.893732 -2.506277 0.511966

CRHTS6b

C -0.583142 -2.068296 0.982299
S 1.047562 -1.733405 0.322947
H -0.832473 -3.115719 0.919864
H -0.592045 -1.751462 2.018947
H -1.310440 -1.468069 0.451935
H -0.190622 1.951039 -1.646879
S -0.766045 1.707114 -0.464371
O 0.582190 1.546704 0.458291
H 0.856345 0.625882 0.439630

H 1.562746 -4.448468 2.386021
H 1.452826 -2.881864 3.171245
H 0.361811 -3.293654 1.836116
H 2.068645 -1.271641 0.935121
S 1.521922 0.140732 0.998766
O 2.724550 0.847597 1.847578
H 2.535656 0.793696 2.778898

RHTS8a

C -1.105643 0.924179 -1.417743
S -0.766917 0.690231 0.318740
O 0.688762 1.396545 0.470204
H 1.349561 0.712682 0.336230
S 0.604325 -1.676600 -0.062256

H	0.378189	-1.957866	1.219589
H	-2.091145	0.511737	-1.592961
H	-1.107244	1.979515	-1.647888
H	-0.382280	0.400834	-2.025363

HTS8a

C	-0.076961	0.101128	-0.200654
S	0.101110	0.067683	1.575154
O	1.647266	-0.127900	1.766494
H	1.982708	-1.149826	1.657126
S	2.452157	-2.810021	1.550253
H	2.067987	-3.056435	2.802839
H	-1.120431	0.302637	-0.406327
H	0.538924	0.882295	-0.622404
H	0.194398	-0.859892	-0.615912

CPHTS8a = CPHTS8b

C	-1.205960	0.950302	-1.458832
S	-1.124006	1.696816	0.169323
O	0.195943	1.311373	0.733663
H	1.240884	-0.687410	0.416065
S	1.492967	-1.914163	-0.044458
H	1.032823	-2.508217	1.053935
H	-2.177719	1.179360	-1.876467
H	-0.427539	1.364386	-2.084398
H	-1.078669	-0.119517	-1.369353

CRHTS8b

C	-0.988276	0.780763	-1.502498
S	-0.795468	0.480626	0.247877
O	0.467940	1.440821	0.601177
H	-1.184956	1.829402	-1.672711
H	-1.842261	0.196481	-1.821635
H	-0.109164	0.470312	-2.048319
H	1.262431	0.908718	0.512369
S	1.117397	-1.581246	0.187907
H	0.852847	-1.714563	-1.111073

HTS8b

C	-0.064451	0.042682	-0.001911
S	0.030157	0.040279	1.780423
O	1.576942	-0.037499	2.042241
H	0.498265	0.872175	-0.405260
H	-1.110447	0.145888	-0.260585
H	0.314203	-0.894110	-0.388175
H	1.977779	-1.039532	2.017870
S	2.552720	-2.669775	1.926533
H	3.564263	-2.384434	1.106291

QCISD/6-311+G(2df,2p) optimized geometries

ch3ssh

H	0.049686	0.120074	0.031564
S	0.006829	-0.043543	1.363746
S	2.038888	-0.020124	1.736240
C	2.357838	1.756336	1.929121
H	3.405932	1.849754	2.212202
H	2.188920	2.284505	0.994453
H	1.732435	2.172113	2.714034

oh

O	0.000000	0.000000	0.000572
H	0.000000	0.000000	0.969428

CRBTS1a = CRFTS1b

S	-0.713050	0.305601	-0.195887
S	-0.451547	-0.056753	1.822742
H	0.568737	0.527943	-0.528632
C	-0.545245	1.621609	2.507645
O	0.842488	-1.739868	-1.808435

H	0.032863	-2.210553	-1.561458
H	-0.491861	1.511489	3.590382
H	0.290533	2.226070	2.165581
H	-1.486362	2.092110	2.237558

BTS1a

S	-0.044692	-0.031037	-0.080885
S	-0.055135	-0.040012	2.017054
H	1.277899	0.058695	-0.237598
C	-0.785303	1.594792	2.333825
O	0.183961	-1.350686	-1.793732
H	-0.696614	-1.747884	-1.803908
H	-0.910171	1.664755	3.413764
H	-0.125333	2.386928	1.991964
H	-1.757949	1.680805	1.857217

CPBTS1a

S	0.283370	-0.153961	-0.073340
S	0.143923	0.044287	2.186997
H	1.177606	-1.113791	0.155145
C	-0.984215	1.463036	2.161749
O	-0.103468	-0.982553	-1.575723
H	-0.715219	-0.406502	-2.043534
H	-0.905811	1.963051	3.124725
H	-0.699342	2.160868	1.376000
H	-2.011427	1.138436	2.016978

CRBTS1b = CRFTS1a

S	0.090919	-0.557173	0.161731
S	-0.034405	-0.044987	2.161301
H	1.279553	-0.000224	-0.116899
O	-0.052048	1.951615	-1.207596
H	-0.891135	1.581649	-1.518355
C	-0.773960	1.611020	2.082493
H	-0.134091	2.293750	1.532443
H	-1.758314	1.569925	1.624526
H	-0.869413	1.942681	3.116168

BTS1b

S	0.118282	0.011489	-0.025311
S	-0.310839	-0.130348	2.007175
H	1.270906	0.662215	0.079663
O	-0.064570	1.242581	-1.738836
H	-0.935159	1.005439	-2.054753
C	-0.665128	1.583695	2.451460
H	0.210401	2.204000	2.331101
H	-1.480102	1.970088	1.858956
H	-0.953201	1.571097	3.494065

CPBTS1b

S	0.130436	0.162004	-0.146581
S	-0.384418	-0.171772	2.037372
H	0.962833	1.131380	0.231025
O	-0.075419	1.041487	-1.663076
H	-0.545369	0.439994	-2.248414
C	-0.598336	1.549423	2.567932
H	0.297110	2.135466	2.366577
H	-1.452604	1.998545	2.067694
H	-0.781782	1.542056	3.640613

FTS1b

H	0.000150	-0.009159	0.142758
S	0.056232	-0.128536	1.483810
S	2.143015	-0.011403	2.121627
C	2.170127	1.786420	2.338948
O	0.490412	-1.878071	1.262239
H	-0.273830	-2.339176	1.623459
H	3.133444	2.021747	2.789541
H	2.089875	2.305864	1.387053
H	1.379398	2.112828	3.010608

CPFTS1b

H	-0.743559	-0.979709	0.175540
S	-0.660309	-0.300029	1.333745
S	3.170600	0.419025	1.506806
C	2.388071	1.702784	2.501805
O	0.423442	-1.278433	2.129063
H	1.308033	-0.955604	1.904053
H	1.872323	1.263594	3.352915
H	3.107819	2.449007	2.824497
H	1.638163	2.174918	1.864705

FTS1a

H	0.256494	0.262357	0.013096
S	-0.026817	0.023875	1.306018
S	1.949423	-0.079799	2.332826
C	2.691736	1.579981	2.378855
O	-0.010622	1.770486	1.717022
H	-0.946127	1.998714	1.692607
H	3.702525	1.431334	2.760656
H	2.746780	2.010685	1.383635
H	2.133465	2.234373	3.038002

CPFTS1a

H	-0.774422	-0.779139	-0.451847
S	-1.918985	-0.161671	-0.104872
S	1.909509	-0.010370	-0.957958
C	1.652839	0.998160	0.514370
O	-1.503473	1.377517	-0.622217
H	-1.792205	1.456661	-1.533495
H	1.411057	0.357789	1.360665
H	2.522052	1.610534	0.736456
H	0.788814	1.635069	0.322015

CBTS2a = CRFTS2b

S	0.141615	0.473861	-0.159527
S	-0.340143	-0.331980	1.680075
C	1.916160	0.147688	-0.269404
H	-0.191483	0.797091	2.393194
O	-0.101906	-1.745378	-1.008679
H	-0.963217	-1.584389	-1.415998
H	2.214661	0.427253	-1.278667
H	2.456321	0.747776	0.457877
H	2.089511	-0.912437	-0.117761

BTS2a

S	-0.013933	0.113012	-0.064750
S	-0.277700	-0.095919	2.000173
C	1.788390	0.062540	-0.177626
H	-0.459245	1.206591	2.270835
O	0.072196	-1.423741	-1.673100
H	-0.866936	-1.649036	-1.687543
H	2.023145	0.185219	-1.231635
H	2.213493	0.871369	0.409395
H	2.150009	-0.901586	0.166265

CPBTS2a

S	-0.007689	-0.076515	-0.199865
S	-0.087156	0.074623	2.162646
C	1.788720	-0.037488	-0.147341
H	-1.424886	0.126941	2.113006
O	0.056118	-1.140851	-1.568902
H	-0.857659	-1.289269	-1.829467
H	2.133227	0.124334	-1.163953
H	2.094722	0.779714	0.496860
H	2.161343	-0.985484	0.232931

CRBTS2b = CRFTS2a = CRPTS3a = CRPTS3b = CRHTS3a

S	0.040571	0.438615	-0.149177
S	-0.375763	-0.129343	1.789065
C	1.799730	0.053930	-0.296912
H	1.945488	-1.011614	-0.151773

H	2.088258	0.327053	-1.310855
H	2.368670	0.636069	0.422484
O	-0.334219	-1.762025	-0.921303
H	-1.120769	-1.556783	-1.442998
H	-0.542930	-1.430363	1.494378

BTS2b

S	-0.074500	0.063988	-0.074882
S	-0.291914	0.146019	1.994944
C	1.710220	-0.046524	-0.246972
H	2.055844	-1.009714	0.095514
H	1.914638	0.055236	-1.301615
H	2.172618	0.751619	0.311451
O	-0.147215	-1.414891	-1.645184
H	-1.087321	-1.582114	-1.684457
H	-0.045277	-1.140097	2.254508

CPBTS2b = CPFTS2a

S	0.130436	0.162004	-0.146581
S	-0.384418	-0.171772	2.037372
H	0.962833	1.131380	0.231025
O	-0.075419	1.041487	-1.663076
H	-0.545369	0.439994	-2.248414
C	-0.598336	1.549423	2.567932
H	0.297110	2.135466	2.366577
H	-1.452604	1.998545	2.067694
H	-0.781782	1.542056	3.640613

FTS2b

C	0.126952	0.108900	-0.067807
S	0.146570	0.229631	1.732101
S	1.954067	-0.729936	2.511924
H	2.606741	0.437675	2.625767
O	-0.496418	-1.493382	1.763156
H	-0.945006	-1.547817	2.613406
H	0.780405	-0.712594	-0.348616
H	-0.887380	-0.096686	-0.397829
H	0.496103	1.046686	-0.475011

CPFTS2b

C	0.026418	0.031569	-0.038571
S	-0.186589	0.221146	1.733873
S	2.506452	-0.058827	2.197821
H	2.292040	0.509054	3.393186
O	-0.321621	-1.349077	2.206465
H	0.584351	-1.636873	2.393966
H	-0.840611	-0.471437	-0.458980
H	0.104184	1.038309	-0.448799
H	0.937046	-0.521351	-0.256502

FTS2a

C	0.097948	-0.044900	-0.025302
S	0.248310	-0.181530	1.762898
S	2.303742	0.603625	2.104371
H	2.008847	1.911131	2.127379
O	-0.266620	1.518984	2.185658
H	-1.174386	1.388439	2.482199
H	-0.124696	0.988915	-0.274086
H	1.031790	-0.352246	-0.489063
H	-0.719219	-0.692358	-0.338148

PTS3a

H	-0.047405	0.020247	-0.038651
S	-0.093845	0.047886	1.440778
S	1.920377	0.024207	1.057983
C	2.278521	-1.730286	0.827862
O	0.954476	-0.024975	-1.082147
H	1.079018	0.864846	-1.434378
H	3.309612	-1.807030	0.487192
H	2.154266	-2.246177	1.776205
H	1.602792	-2.124286	0.075565

CPPTS3a = CPPTS3b = CPHTS3 = CHHTS3b

H	-0.713506	0.300795	-1.633540
S	-0.768441	0.854969	0.833193
S	0.641541	-0.370415	1.471364
C	1.239466	-1.244117	-0.004722
O	-0.456628	-0.114663	-2.462034
H	-1.016858	0.288599	-3.124621
H	2.019181	-1.924509	0.333759
H	0.426266	-1.799347	-0.462121
H	1.642978	-0.532825	-0.718896

PTS3b

H	-0.024545	-0.066502	-0.008191
S	0.025388	-0.028318	1.464570
S	2.016377	-0.036563	1.003907
C	2.390160	-1.800085	0.852569
O	0.902905	0.090195	-1.106284
H	1.111529	-0.664683	-1.670932
H	3.386184	-1.889580	0.421829
H	2.367477	-2.258289	1.837983
H	1.651648	-2.268047	0.208050

HTS3a

H	-0.177620	-0.023542	0.107673
S	-0.111946	0.107686	1.478335
S	1.930623	0.081668	1.684331
C	2.299523	-1.689229	1.535435
O	-0.087703	0.499208	-1.429925
H	0.391174	1.325132	-1.259874
H	3.371443	-1.795579	1.698430
H	1.757552	-2.252675	2.289589
H	2.046774	-2.046947	0.540872

HTS3b

H	0.026459	0.134588	-0.013614
S	-0.051312	0.174682	1.366975
S	1.951929	0.074941	1.795024
C	2.227591	-1.717251	1.864903
O	0.086226	-0.745761	-1.358926
H	-0.432217	-1.516865	-1.082954
H	3.264490	-1.858407	2.167874
H	1.568751	-2.176558	2.596531
H	2.073830	-2.158042	0.883199

CRTS11a

S	-0.044042	0.222402	-0.079796
S	0.080267	-0.351022	1.903922
C	1.683531	0.103483	-0.625221
H	2.070703	-0.900303	-0.477778
H	1.673955	0.336488	-1.689573
H	2.303903	0.829445	-0.106018
H	0.421816	0.831659	2.441768
O	3.032101	-2.184594	1.789695
H	2.185243	-1.733065	1.950074

HTS11a

S	-0.008422	-0.028286	-0.014051
S	-0.041608	-0.087819	2.053094
C	1.741663	-0.011751	-0.344754
H	2.245786	-1.013849	0.090941
H	1.896742	-0.048610	-1.421732
H	2.263902	0.822056	0.114846
H	0.091843	1.228054	2.286342
O	2.823067	-2.005475	0.760318
H	2.447107	-1.788196	1.626050

CPHTS11a = CPHTS11b

S	0.014386	-0.200295	0.223172
S	0.044997	0.439366	2.195024
C	1.535310	0.335033	-0.378666

H	2.790481	-1.478551	0.557480
H	1.791784	0.006545	-1.375235
H	2.059031	1.149584	0.095013
H	-0.556737	1.621535	1.991058
O	3.304452	-2.230401	0.860571
H	2.647843	-2.880145	1.110833

HTS11b

S	0.093401	-0.188885	-0.012758
S	0.116496	-0.120002	2.054466
C	1.809353	0.062404	-0.424156
H	2.469062	-0.891814	-0.131575
H	1.894520	0.167055	-1.503967
H	2.260716	0.896124	0.106176
H	-0.053636	1.204826	2.189915
O	3.155480	-2.022547	0.109213
H	2.379905	-2.600931	0.142461

CH3S

C	0.001682	0.006259	0.003091
S	-0.001241	-0.006323	1.805332
H	1.013703	-0.002943	-0.392984
H	-0.498956	-0.910679	-0.314474
H	-0.557860	0.851965	-0.388134

CH3SS

C	-0.003308	-0.002238	0.005356
S	-0.018319	-0.039931	1.822469
S	1.881823	0.040149	2.342303
H	0.463050	0.917877	-0.335568
H	-1.039043	-0.042752	-0.328640
H	0.543992	-0.861766	-0.371627

CH3SOH

C	-0.004768	-0.002716	0.011200
S	0.027295	-0.017307	1.809729
H	1.037189	0.020722	-0.310113
H	-0.479384	-0.896152	-0.388907
H	-0.510353	0.889534	-0.350038
O	-1.610438	0.076940	2.127949
H	-1.939063	-0.820937	2.208294

HSOH

H	0.027629	-0.041344	0.004636
S	-0.020391	0.030211	1.346375
O	1.623964	0.024353	1.643785
H	1.884798	-0.889097	1.774675

SH

S	0.012212	-0.020348	0.000518
H	-0.105883	-0.168878	1.329469

CH2SSH

C	0.001362	0.051182	-0.001796
S	0.007451	0.102186	1.715014
H	0.920251	0.079072	-0.563260
H	-0.961034	0.111072	-0.485470
S	1.860391	-0.697710	2.205133
H	2.522866	0.465263	2.299828

Reactions starting by HSSNH₂ + OH

BH&HLYP/6-311+G(2df,2p) optimized geometries

HSSNH2

H	0.068620	0.119074	0.036732
S	0.031453	-0.018263	1.371953

S	2.081833	-0.027873	1.732971
N	2.577871	1.566986	1.944436
H	2.158185	2.020346	2.741468
H	2.490088	2.135753	1.116560

SSNH2

S	-0.004329	-0.005380	-0.001176
S	0.003513	0.005687	1.949198
N	1.569398	0.001436	-0.597687
H	2.085914	-0.815297	-0.327930
H	2.073504	0.830295	-0.341920

SNH2

N	-0.004327	0.008705	0.003367
S	0.004461	-0.002240	1.627064
H	0.842808	-0.003120	-0.523212
H	-0.857045	0.028450	-0.513887

HSNH2

S	0.000553	-0.000146	0.003030
N	-0.019235	-0.000062	1.701910
H	1.324141	0.000162	-0.164661
H	-0.450787	-0.823130	2.070941
H	-0.451190	0.822834	2.070854

OSNH2

N	0.000181	0.002059	-0.001446
S	0.003820	-0.058409	1.661502
O	1.376234	0.067586	2.185044
H	0.483417	-0.763240	-0.435666
H	0.308525	0.881111	-0.375535

CRFTS1a = CRBTS1a

H	-1.180796	0.279750	-1.353982
S	-1.138356	0.234730	-0.021408
S	0.921048	0.162344	0.245636
N	1.463064	1.720618	0.432866
O	-0.811396	-2.424279	-0.682850
H	-1.377643	-2.610945	0.069110
H	1.160621	2.195101	1.259611
H	1.423469	2.300359	-0.381036

FTS1a

H	-0.235094	0.044954	0.250922
S	0.061825	-0.076173	1.549904
S	2.259485	-0.023823	1.842076
N	2.555331	1.571225	2.122651
O	0.454372	-1.816613	1.214865
H	-0.119492	-2.315396	1.789996
H	2.233760	1.964305	2.982531
H	2.513694	2.199078	1.347193

CPFTS1a

H	-2.549259	-0.104318	0.358368
S	-1.851734	-0.066131	-0.782886
S	1.666216	-0.088862	0.827179
N	1.112197	1.380136	0.424264
O	-0.992950	-1.451705	-0.620133
H	-0.172360	-1.250631	-0.160621
H	0.211281	1.487378	-0.000146
H	1.649311	2.201759	0.604005

CRFTS1b = CRBTS1b

H	-0.868969	-0.756721	-1.623304
S	-0.836952	-1.087715	-0.330122
S	1.130104	-0.671619	0.059749
N	1.136847	0.972096	0.484783
O	-1.512920	2.389051	0.134942
H	-0.718636	1.851740	0.274841
H	1.410370	1.115337	1.438182
H	1.699139	1.519764	-0.138492

FTS1b

H	-0.114456	0.099293	0.033533
S	-0.079717	-0.108291	1.353636
S	2.024510	-0.039415	1.851542
N	2.491091	1.549202	2.155748
O	-0.306298	1.646632	1.678239
H	0.561878	2.044255	1.791422
H	2.717784	1.751719	3.109511
H	3.142268	1.933934	1.500759

CPFTS1b = CPBTS1a

H	-1.636403	-0.997340	-0.512642
S	-1.844998	0.250059	-0.077242
S	2.445420	-0.140657	-0.027372
N	1.422676	0.933482	0.656252
O	-1.050099	1.073319	-1.255914
H	-0.131507	1.156203	-1.006135
H	0.578320	0.614594	1.093177
H	1.761274	1.826101	0.951559

BTS1b

S	-0.012054	0.035611	0.010108
N	-0.103411	-0.013887	1.668840
S	2.042858	0.021344	-0.445863
H	2.280431	-1.244489	-0.128069
H	-0.450087	0.808895	2.114443
H	-0.426666	-0.869320	2.068377
O	4.017908	0.274446	0.210000
H	4.105146	1.226279	0.220003

BTS1a

S	-0.100589	-0.237476	-0.038046
N	-0.258949	0.054745	1.588569
S	1.997862	-0.245162	-0.439096
H	2.092380	-1.544512	-0.683332
H	-0.072834	0.989469	1.890741
H	0.119850	-0.637761	2.202607
O	3.532272	-0.128309	-1.798190
H	3.585784	0.807551	-1.983202

CRFTS2a

N	-0.656558	0.540835	-1.536836
S	-0.615901	0.546283	0.114330
S	1.313538	0.148003	0.752993
H	1.716786	1.415552	0.869464
O	-0.768069	-1.876609	-0.213009
H	-1.507091	-2.026059	0.376882
H	-0.498340	-0.364793	-1.935712
H	-0.153257	1.278945	-1.986348

FTS2a

N	-0.037038	0.171527	-0.113192
S	0.073461	0.099605	1.543963
S	2.066349	-0.221964	2.361367
H	2.248911	1.072069	2.624711
O	0.051330	-1.660944	1.327678
H	-0.253764	-2.013337	2.159405
H	-0.565681	-0.557667	-0.551109
H	-0.191727	1.096665	-0.455526

CPFTS2a

N	-0.653377	0.655678	-1.601767
S	-1.045034	0.222148	-0.083504
S	1.613374	0.319239	0.647632
H	1.243134	0.823792	1.822055
O	-0.921513	-1.396405	0.023782
H	-0.026488	-1.610387	0.294060
H	-1.298276	0.424219	-2.329465
H	0.312348	0.638604	-1.863061

CRFTS2b

N	-0.763221	-0.318859	-1.547821
S	-0.531535	-0.613602	0.061817
S	1.432055	-0.205853	0.559770
H	1.272400	1.105709	0.751522
O	-1.032493	1.751321	0.260377
H	-1.812347	1.677919	0.810247
H	-0.729504	0.654877	-1.781868
H	-0.246331	-0.906384	-2.171171

FTS2b

N	-0.202644	0.061779	-0.063605
S	0.188973	-0.103179	1.548226
S	2.289915	0.207650	2.233007
H	2.317805	1.538493	2.261239
O	-0.064639	1.635216	1.719082
H	-0.475558	1.750995	2.571449
H	-0.361182	1.008723	-0.352651
H	0.429257	-0.430806	-0.663817

CPFTS2b = CPBTS2a = CPBTS2b

N	-0.628054	-0.443333	-1.572186
S	-1.022992	-0.290811	-0.005393
S	1.828344	-0.240429	0.552481
H	1.479034	0.962354	1.007849
O	-1.114054	1.323233	0.320593
H	-2.010662	1.625232	0.211055
H	-1.329572	-0.298059	-2.268125
H	0.308849	-0.203225	-1.831936

CRBTS2a

S	-0.025514	0.442252	0.183003
N	0.015756	0.141581	1.804379
S	1.726454	-0.305741	-0.594603
H	1.311255	-1.570194	-0.699784
H	0.059599	0.940293	2.400142
H	-0.580164	-0.606342	2.096751
O	-1.113566	-1.686797	0.128259
H	-1.769674	-1.482058	-0.537326

BTS2a

S	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.661983
S	2.026965	0.000000	-0.567617
H	2.300946	-1.252144	-0.225804
H	-0.334474	0.831191	2.101260
H	-0.287790	-0.847172	2.103987
O	-1.707779	-1.099877	0.518460
H	-2.026285	-1.389325	-0.335045

CRBTS2b

S	0.108381	-0.196457	0.231670
N	-0.196433	0.130213	1.817062
S	2.146750	-0.001020	-0.023715
H	2.474189	-1.275906	0.198212
H	-0.577191	1.037481	1.992691
H	-0.540382	-0.622639	2.372711
O	-0.173885	2.215934	0.054834
H	-0.509243	2.229470	-0.841524

BT2b

S	0.284538	0.166920	0.156122
N	0.004199	0.215923	1.797065
S	2.347743	-0.327580	0.151689
H	2.207035	-1.329470	-0.716268
H	-0.421325	1.093102	2.032670
H	-0.542025	-0.562024	2.111852
O	-0.902497	1.860865	0.037296
H	-0.652842	2.261455	-0.792284

RHTS3b

S	-0.461678	-0.109815	-0.605150
S	-0.204419	-1.343089	1.032505
N	0.995829	0.132719	-1.346218
H	1.417488	-0.683512	-1.742380
H	1.625373	0.697447	-0.808808
H	0.150231	-0.384660	1.891587
O	0.252216	1.771434	0.751665
H	-0.456859	2.373383	0.526250

HTS3b

S	-0.056193	0.205981	0.118106
S	-0.030799	-0.183169	2.130961
N	1.506426	0.158712	-0.452885
H	1.957311	-0.732337	-0.385918
H	2.094819	0.904818	-0.138495
H	0.286177	1.073368	2.608309
O	0.127036	2.533853	3.157082
H	-0.811712	2.676635	3.012851

CPHTS3b

S	-0.276117	-0.685438	-1.084474
S	-0.621391	-1.192097	0.772700
N	0.949730	0.448610	-1.183921
H	1.855539	0.040358	-1.043321
H	0.815328	1.226464	-0.556577
H	0.151109	1.185352	1.659964
O	0.491172	2.010956	1.323799
H	-0.020324	2.701756	1.726920

CRHTS3a

S	-0.133915	-1.017645	-0.744323
S	-0.453470	-0.305348	1.184283
N	0.975673	-0.029802	-1.485595
H	1.904274	-0.097466	-1.118546
H	0.688501	0.925197	-1.581732
H	-1.478564	0.510459	0.933041
O	0.253672	2.392685	0.406169
H	0.832377	2.301146	1.167102

HTS3a

S	0.047775	-0.408256	0.060490
S	0.129664	0.194656	2.017192
N	1.559935	-0.244360	-0.614597
H	2.271887	-0.826141	-0.219630
H	1.866319	0.699826	-0.742204
H	-0.172586	1.536200	1.856359
O	0.072047	3.071813	1.724302
H	0.895269	3.178206	2.207071

CPHTS3a

S	-0.063354	-1.189571	-0.605878
S	-0.382082	-0.841928	1.292077
N	0.982829	-0.059935	-1.260056
H	1.935027	-0.224121	-0.989276
H	0.716778	0.889168	-1.047440
H	-0.412527	3.100149	0.328824
O	0.214816	2.389708	0.273249
H	-0.006392	1.773125	0.966797

CROTS3a

H	-1.697984	0.146890	-0.726519
S	-1.437653	0.217551	0.580984
S	0.610174	0.294241	0.398228
N	1.123164	-1.264901	0.231165
O	0.530539	0.201568	-1.991715
H	0.861400	1.081915	-2.167720
H	1.398522	-1.507387	-0.699103
H	1.684202	-1.625419	0.972890

PTS3a

H	0.062642	-0.021943	-0.141258
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S	-0.284547	-0.055562	1.284029
S	1.732811	-0.008169	1.385972
N	2.239125	-1.582764	1.200602
O	1.282868	-0.046323	-0.924227
H	1.498541	0.775628	-1.357592
H	2.224987	-1.859722	0.234487
H	3.132049	-1.731481	1.631209

CPPTS3a

H	-0.490867	0.281420	-1.937366
S	-1.233009	0.487153	0.525033
S	0.408600	-0.194213	1.282821
N	1.155381	-1.152857	0.129463
O	0.253986	-0.011978	-2.458818
H	0.490419	0.712085	-3.025568
H	1.053921	-0.817885	-0.818514
H	2.113499	-1.321248	0.376035

CRHTS5a

H	-1.775108	0.950203	-1.537154
S	-1.475020	1.213740	-0.260113
O	0.090814	1.660851	-0.438891
H	0.642842	0.876847	-0.364171
S	1.415159	-1.338058	0.071739
N	-0.017454	-1.859794	0.622181
H	-0.122449	-2.777801	0.999171
H	-0.825935	-1.269971	0.581026

HTS5a

H	-0.264975	-0.779272	0.534139
S	0.202731	-0.127594	1.614884
O	1.700573	0.038476	1.262368
H	2.392191	-0.949309	1.604949
S	2.885694	-2.315544	2.109815
N	1.345521	-2.893615	2.404649
H	1.027409	-3.639377	1.821201
H	1.077892	-2.992135	3.361794

CPHTS5a = CPHTS5b

N	-0.737510	-1.439322	1.178577
S	-0.124463	-2.214975	-0.223667
H	-1.707369	-1.655601	1.304886
H	-0.225243	-1.724324	1.990805
H	0.232495	-1.112729	-0.884516
O	0.465103	1.242717	-1.137474
S	-0.063842	1.950790	0.070016
H	-0.480240	0.932056	0.861832

CRHTS5b

N	-0.983841	-2.097560	0.800773
S	0.628944	-2.175960	0.655465
H	-1.523645	-2.905586	1.026384
H	-1.466622	-1.229008	0.679588
H	0.254238	0.196995	0.267559
O	-0.507681	0.780483	0.280807
S	-0.324425	1.965700	-0.849587
H	0.247002	2.891464	-0.072979

HTS5b

N	1.367254	-2.995386	2.482440
S	2.747785	-2.221444	1.997615
H	1.052167	-3.771509	1.941782
H	1.178687	-3.051392	3.459799
H	2.159469	-0.931968	1.461479
O	1.697385	0.167909	1.017828
S	2.782969	1.231757	0.678648
H	2.920543	1.857160	1.861903

CRHTS6a 0 CRHTS6b

H	-1.039679	1.456280	-1.192823
O	-1.269090	1.017446	-0.380402

S	-0.323281	1.624739	0.842132
H	0.702418	0.775843	0.709874
S	1.018747	-1.848043	-0.598151
N	-0.601109	-1.908306	-0.539364
H	-1.085340	-2.780104	-0.563965
H	-1.142354	-1.069048	-0.459776

HTS6a

H	-0.201416	-0.433040	0.327804
O	0.122909	-0.046990	1.135876
S	1.731647	0.200628	0.998714
H	2.165301	-1.330980	1.355847
S	2.129082	-2.868985	1.533697
N	0.796272	-3.165984	0.591752
H	0.954985	-3.639997	-0.272538
H	-0.030686	-3.452309	1.072408

CPHTS6a

H	-1.074022	0.275404	-0.484538
O	-1.251446	1.231932	-0.525798
S	0.004610	2.046842	0.053700
H	1.219286	-0.592793	0.487003
S	0.860508	-1.860688	0.281091
N	-0.691953	-1.521609	-0.385782
H	-0.754389	-1.885191	-1.318463
H	-1.408733	-1.942223	0.175728

HTS6b

N	0.232895	0.123766	0.370619
S	-0.660357	-0.290918	1.691993
H	0.948056	0.808641	0.506459
H	-0.254346	0.216711	-0.496565
H	-1.434299	1.008877	1.942592
S	-1.805232	2.621635	2.009260
O	-0.247894	3.128852	1.911004
H	0.104835	3.227310	2.789813

CPHTS6b

N	1.228843	-1.241774	-1.411301
S	0.481328	-1.171161	0.093095
H	1.009228	-0.484520	-2.026039
H	1.149919	-2.128781	-1.865604
H	-0.823380	-1.250416	-0.208710
S	-1.197464	2.219716	1.263749
O	0.313157	2.029674	0.744292
H	0.478528	1.094911	0.567962

CRHTS8a = CRHTS8b

N	-1.154342	0.687651	-1.252827
S	-0.733064	0.712865	0.318150
O	0.685687	1.499264	0.444395
H	1.392139	0.855856	0.362022
S	0.747573	-1.590357	-0.023831
H	0.341614	-1.994860	1.177110
H	-0.668478	0.059529	-1.861563
H	-1.442965	1.549769	-1.668114

HTS8a

N	0.232895	0.123766	0.370619
S	-0.660357	-0.290918	1.691993
H	0.948056	0.808641	0.506459
H	-0.254346	0.216711	-0.496565
H	-1.434299	1.008877	1.942592
S	-1.805232	2.621635	2.009260
O	-0.247894	3.128852	1.911004
H	0.104835	3.227310	2.789813

CPHTS8a

N	-1.175719	0.729190	-1.268911
S	-1.052828	1.581524	0.148652
O	0.339308	1.576236	0.642611

H	1.361931	-0.632965	0.448778
S	1.230119	-1.834782	-0.114184
H	0.667541	-2.369569	0.967059
H	-0.820707	-0.210528	-1.201758
H	-0.791936	1.205806	-2.064710

HTS8b

S	0.061257	0.006055	-0.008662
N	0.003876	-0.092029	1.624719
H	0.882249	-0.082324	2.105919
H	-0.703256	0.455491	2.077106
O	0.757790	1.357754	-0.387167
H	0.091183	2.215349	-0.407890
S	-1.034033	3.514474	-0.385804
H	-0.248800	4.316881	0.333200

CPHTS8b

S	0.564578	-1.732350	-0.028561
N	0.086035	-1.160261	1.453410
H	0.840946	-1.037284	2.103544
H	-0.482592	-0.331395	1.395724
O	1.259618	-0.678379	-0.795423
H	0.050366	1.460834	-0.661674
S	-0.983405	2.059076	-0.068255
H	-0.206327	2.879761	0.634866

QCISD/6-311+G(2df,2p) optimized geometries

HSSNH2

H	0.068620	0.119074	0.036732
S	0.031453	-0.018263	1.371953
S	2.081833	-0.027873	1.732971
N	2.577871	1.566986	1.944436
H	2.158185	2.020346	2.741468
H	2.490088	2.135753	1.116560

SNH2

N	-0.004318	0.004182	0.000812
S	0.004395	-0.001209	1.638192
H	0.848875	-0.001481	-0.527679
H	-0.863056	0.030304	-0.517992

OHSNH2

S	-0.003462	0.027126	-0.032400
O	-0.001224	-0.013861	1.642741
H	0.913469	-0.007457	1.933837
N	-0.003648	-1.546055	-0.535766
H	0.845531	-2.071904	-0.411589
H	-0.835764	-2.079144	-0.343343

SSNH2

S	-0.015905	-0.005924	-0.012256
S	0.015783	0.006323	1.955490
N	1.573762	0.001323	-0.623067
H	2.083438	-0.815776	-0.313482
H	2.070923	0.830795	-0.326200

CRFTS1a = CRBTS1a

S	0.180856	0.160244	-0.047741
N	-0.484654	-0.183361	1.457783
S	2.237453	0.389799	0.203646
H	2.604908	-0.890393	0.030862
H	-0.372017	0.555839	2.134367
H	-0.203051	-1.073540	1.838537
O	3.544159	-0.586254	-2.409510
H	3.302625	0.337138	-2.574587

FTS1a

H	-0.226738	0.064973	0.260466
S	0.081973	-0.075457	1.563665
S	2.294489	-0.043385	1.848348
N	2.585227	1.575127	2.124967
O	0.465946	-1.817883	1.216064
H	-0.144582	-2.301031	1.781779
H	2.196172	1.957902	2.971065
H	2.471392	2.187311	1.333784

CPFTS1a

H	-2.549928	-0.118559	0.380703
S	-1.843341	-0.071780	-0.764166
S	1.645305	-0.069940	0.892092
N	1.102556	1.383070	0.375237
O	-0.963648	-1.466840	-0.588969
H	-0.154871	-1.231724	-0.109899
H	0.196470	1.465100	-0.057649
H	1.640158	2.218298	0.522679

CRFTS1b = CRBTS1b

S	-0.009419	-0.291961	0.153285
N	0.750710	0.313719	1.569749
S	1.485894	-0.215703	-1.261908
H	2.043892	-1.413713	-1.023106
H	0.321200	1.178186	1.867846
H	0.709198	-0.368019	2.314489
O	3.765363	0.628804	1.319035
H	2.790949	0.581673	1.315692

FTS1b

H	-0.105578	0.098091	0.017114
S	-0.100223	-0.110392	1.345548
S	2.020113	-0.043619	1.860615
N	2.470530	1.578181	2.149408
O	-0.313645	1.650377	1.697546
H	0.580871	2.019089	1.797003
H	2.726382	1.760158	3.108617
H	3.158609	1.925442	1.498540

CPFTS1b = CPBTS1b = CPBTS1a

H	-1.506067	-1.017489	-0.608548
S	-1.808887	0.112858	0.055997
S	2.329351	-0.077147	-0.413087
N	1.437881	0.912068	0.562233
O	-1.189698	1.215856	-1.023550
H	-0.258461	1.331145	-0.803369
H	0.663020	0.520875	1.077258
H	1.877543	1.717597	0.974749

BTS1**b**

S	-0.037967	-0.047183	0.000819
N	0.001188	0.023558	1.691104
S	1.980431	-0.007372	-0.551374
H	2.270700	-1.279375	-0.261251
H	-0.429572	0.856358	2.058928
H	-0.353841	-0.810872	2.129496
O	4.030432	0.275140	0.249070
H	3.992755	1.228626	0.401046

BTS1**a**

S	-0.089400	-0.159325	-0.068480
N	-0.308054	0.044279	1.586628
S	2.012548	-0.183993	-0.383858
H	2.132854	-1.502739	-0.554213
H	-0.025952	0.946277	1.937632
H	0.057688	-0.706243	2.151820
O	3.558130	-0.159876	-1.854004
H	3.557962	0.780166	-2.075473

CRFTS2a

N	-0.691599	0.529713	-1.547245
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S	-0.637020	0.504832	0.119896
S	1.309798	0.104785	0.734142
H	1.683216	1.388880	0.867351
O	-0.712135	-1.788068	-0.191855
H	-1.486125	-1.963841	0.357783
H	-0.488805	-0.382264	-1.933372
H	-0.146222	1.268120	-1.964936

FTS2a

N	-0.004141	0.155713	-0.160399
S	0.084266	0.102433	1.528077
S	2.069257	-0.239774	2.387424
H	2.238142	1.063318	2.659463
O	0.050911	-1.659439	1.315555
H	-0.211008	-1.991227	2.180406
H	-0.629124	-0.539602	-0.544594
H	-0.206462	1.094532	-0.468636

CPFTS2a

N	-0.647828	0.690570	-1.594573
S	-1.056957	0.232290	-0.069098
S	1.597697	0.295800	0.628079
H	1.233704	0.822112	1.804792
O	-0.930443	-1.407386	0.017401
H	-0.020795	-1.594271	0.289218
H	-1.279620	0.410029	-2.326941
H	0.328411	0.627744	-1.839147

CRFTS2b

N	-0.795972	-0.305696	-1.550322
S	-0.562638	-0.580666	0.079707
S	1.419028	-0.196177	0.562573
H	1.246625	1.126061	0.729878
O	-0.986474	1.685511	0.249215
H	-1.784034	1.637657	0.790965
H	-0.710246	0.676492	-1.773187
H	-0.237266	-0.898054	-2.145956

FTS2b

N	-0.228990	0.050430	-0.079796
S	0.185646	-0.111112	1.552173
S	2.285513	0.206597	2.286412
H	2.304215	1.544646	2.222991
O	-0.065763	1.633609	1.707082
H	-0.442087	1.742043	2.585854
H	-0.363896	1.014684	-0.351812
H	0.447290	-0.412024	-0.669974

CPFTS2b = CPBTS2a = CPBTS2b

S	-0.522591	0.383556	0.258877
N	-0.175579	0.335308	1.863309
S	2.376382	-0.345883	-0.110319
H	1.711190	-1.395464	-0.617329
H	-0.937225	0.194363	2.505571
H	0.684779	-0.128511	2.112517
O	-0.862054	-1.185493	-0.212827
H	-1.810741	-1.318369	-0.143868

CRBTS2a

S	-0.045256	0.421356	0.182117
N	0.066562	0.110419	1.826336
S	1.700215	-0.321642	-0.627078
H	1.262541	-1.590824	-0.687676
H	-0.013138	0.946820	2.382265
H	-0.581491	-0.618774	2.089346
O	-1.053653	-1.628591	0.148831
H	-1.711634	-1.445771	-0.533319

BTS2a

S	-0.072355	0.149775	0.119290
N	0.128937	0.059808	1.791904

S	1.896793	-0.043078	-0.574967
H	2.019057	-1.354687	-0.313293
H	-0.149497	0.927253	2.227310
H	-0.437175	-0.705930	2.134559
O	-1.633531	-1.242553	0.387663
H	-1.780646	-1.547915	-0.515242

CRBTS2b

S	0.090399	-0.169850	0.242219
N	-0.152225	0.148182	1.869965
S	2.121947	0.067927	-0.053905
H	2.454829	-1.217740	0.148706
H	-0.585677	1.052265	1.994282
H	-0.628814	-0.603572	2.341551
O	-0.111874	2.101075	0.080008
H	-0.456399	2.138789	-0.820885

BTS2b

S	0.277242	0.190008	0.116907
N	0.029964	0.182756	1.785058
S	2.356246	-0.219719	0.015847
H	2.207557	-1.436715	-0.530219
H	-0.382742	1.070055	2.042291
H	-0.580662	-0.577895	2.046522
O	-0.908164	1.889765	0.075860
H	-0.674616	2.280935	-0.774124

CRHTS3a

S	-0.175335	-0.994061	-0.790826
S	-0.449449	-0.366956	1.185431
N	1.002065	-0.015784	-1.481648
H	1.917032	-0.149078	-1.078304
H	0.754750	0.963263	-1.486442
H	-1.431107	0.523066	0.968354
O	0.189299	2.408386	0.341525
H	0.781292	2.310390	1.102308

HTS3a

S	0.019638	-0.432375	0.097942
S	0.055648	0.146150	2.081161
N	1.531867	-0.094886	-0.557802
H	2.285170	-0.610788	-0.128411
H	1.733624	0.894412	-0.579017
H	-0.285687	1.482842	1.894575
O	0.297788	2.867623	1.426641
H	1.032261	2.948966	2.053894

CPHTS3a

S	-0.299642	-0.668198	-1.090556
S	-0.602420	-1.194543	0.787338
N	0.959012	0.457243	-1.206327
H	1.851079	0.021151	-1.012734
H	0.820567	1.233000	-0.565803
H	0.153833	1.179791	1.647528
O	0.499995	2.015444	1.321928
H	-0.037378	2.692074	1.733716

HTS3b

S	-0.101869	0.237006	0.167743
S	-0.025378	-0.263977	2.170386
N	1.471185	0.233208	-0.432999
H	1.920925	-0.668366	-0.377935
H	2.054212	0.952523	-0.031781
H	0.325147	0.971175	2.676103
O	0.159853	2.514459	3.116038
H	-0.731011	2.661832	2.762457

CPHTS3b

S	-0.299642	-0.668198	-1.090556
S	-0.602420	-1.194543	0.787338
N	0.959012	0.457243	-1.206327

H	1.851079	0.021151	-1.012734
H	0.820567	1.233000	-0.565803
H	0.153833	1.179791	1.647528
O	0.499995	2.015444	1.321928
H	-0.037378	2.692074	1.733716

CRPTS3a

H	-1.664976	0.148130	-0.767111
S	-1.438284	0.251164	0.553514
S	0.615431	0.297093	0.370163
N	1.079148	-1.308463	0.229550
O	0.517016	0.175595	-1.909358
H	0.835957	1.064899	-2.107115
H	1.390013	-1.501674	-0.712202
H	1.738059	-1.582287	0.940769

PTS3a

H	0.060091	-0.045457	-0.137378
S	-0.302137	-0.031247	1.292034
S	1.731500	0.011375	1.359772
N	2.220177	-1.591041	1.187523
O	1.306999	-0.088545	-0.900487
H	1.504040	0.762713	-1.306033
H	2.240495	-1.829816	0.202255
H	3.127312	-1.718319	1.615533

CPPTS3a

H	-0.501239	0.228784	-1.939494
S	-1.267687	0.455078	0.519185
S	0.464783	-0.074612	1.231747
N	1.134500	-1.185860	0.131007
O	0.267226	-0.006119	-2.469014
H	0.471683	0.779470	-2.976405
H	1.090647	-0.839474	-0.825008
H	2.092019	-1.374791	0.401067

Reactions starting by HSSCOOH + OH

BH&HLYP/6-311+G(2df,2p) optimized geometries

HSSCOOH

C	0.000986	0.004234	0.008353
S	0.007963	-0.022030	1.792328
S	2.005145	-0.006387	2.218394
H	2.189743	1.314375	2.195090
O	0.932386	0.106162	-0.709800
O	-1.263756	-0.099275	-0.388985
H	-1.281583	-0.071277	-1.345018

SSCOOH

S	0.012904	0.000085	0.022541
C	-0.005461	-0.000613	1.771988
O	0.990043	0.000315	2.417481
O	-1.235104	-0.002398	2.264472
H	-1.177024	-0.002745	3.220391

SSCOOH

C	0.000524	-0.000013	0.005071
O	-0.000942	-0.000019	1.181565
O	1.073564	0.000003	-0.774522
H	1.855109	0.000009	-0.221816
S	-1.451908	-0.000023	-1.075882
S	-2.969891	-0.000038	0.154353

HSSCOOH

C	0.002951	0.000022	0.010281
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O	-0.010282	0.000078	1.194820
O	1.105804	-0.000127	-0.731368
H	1.858805	-0.000179	-0.141757
S	-1.411070	0.000121	-1.046818
H	-2.270189	0.000257	-0.031704

OSCOOH

C	0.004458	0.000014	-0.003057
O	-0.002020	-0.000010	1.322585
H	0.900149	-0.000022	1.643362
O	0.948131	0.000022	-0.704876
S	-1.719928	0.000036	-0.577906
O	-1.614111	0.000060	-2.053671

CRBTS1a

S	0.215755	-0.411017	0.310626
S	0.405139	-0.519709	2.351362
C	1.808729	0.043691	-0.330911
H	0.102651	0.745820	2.639247
O	-1.912169	-0.259749	4.000711
H	-2.171807	-1.154170	3.765550
O	1.960091	0.108041	-1.505271
O	2.739206	0.294404	0.571581
H	3.542959	0.524462	0.105565

BTS1a

S	0.077335	-0.104750	0.101553
S	-0.051087	-0.079368	2.205685
C	1.809058	0.002217	-0.270763
H	-0.658881	1.097270	2.265100
O	-1.311641	-0.491948	3.810563
H	-1.205842	-1.434781	3.932911
O	2.167545	-0.010673	-1.400407
O	2.609348	0.085231	0.778281
H	3.509574	0.129638	0.455888

CPBTS1a

S	1.136819	-0.099329	-0.571904
C	1.158166	-0.107919	1.185459
O	2.164805	-0.110850	1.814349
O	-0.053344	-0.117959	1.746771
H	0.076297	-0.119115	2.694859
S	-1.186146	0.425962	-0.979395
H	-0.803129	0.467343	-2.248491
O	-2.709859	-0.134495	-1.442788
H	-3.268202	-0.146914	-0.669975

CRBTS1b = CRFTS1b

S	-0.613489	0.528661	-0.222519
S	-0.458433	0.157673	1.781975
H	0.685070	0.657351	-0.493499
C	-0.469626	1.805865	2.465658
O	0.509946	-1.627196	-1.774352
H	-0.336637	-2.068687	-1.670026
O	-0.464482	1.689386	3.789736
O	-0.470360	2.825945	1.871901
H	-0.454018	2.567508	4.169217

BTS1b

S	0.060319	0.111054	-0.021716
S	0.061316	0.090847	2.076728
H	1.351958	-0.168779	-0.124806
C	-0.514283	1.742811	2.406433
O	-0.042708	-1.127594	-1.727961
H	-0.985561	-1.239313	-1.846483
O	-0.589508	1.891975	3.724678
O	-0.797352	2.571222	1.613147
H	-0.908469	2.775299	3.908118

CPBTS1b

S	0.014822	-0.819103	0.083188
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C	0.274783	-0.015912	1.597920
O	1.327415	0.404239	2.010537
O	-0.838186	0.102299	2.303850
H	-0.621959	0.541757	3.126534
S	2.782033	-0.554006	-0.808043
H	2.480912	0.631289	-1.356006
O	3.480791	-0.073958	0.558870
H	2.780320	0.142165	1.203044

CRFTS1a = CRHTS3a = CRHTS3b

H	0.315427	0.117753	0.403265
S	0.297316	-0.281483	1.676026
S	2.309181	-0.212408	2.029747
C	2.567439	1.486270	2.481490
O	-0.575317	2.700074	0.780275
H	0.151249	2.698291	1.418149
O	3.827756	1.623722	2.861674
O	1.777801	2.372385	2.447883
H	3.982645	2.541646	3.083856

FTS1a

H	-0.273933	-0.237156	0.313960
S	0.053868	0.084089	1.578093
S	2.200612	0.111110	1.711843
C	2.565864	1.634373	2.540062
O	0.016586	1.757833	0.858646
H	0.220532	2.349558	1.583657
O	3.875013	1.706898	2.736382
O	1.790589	2.458307	2.904697
H	4.063302	2.516661	3.211428

CPFTS1a

H	0.241993	0.077487	0.048176
S	-0.281193	0.085904	1.281940
S	2.397805	-0.204151	2.402405
C	2.704680	1.500457	2.484321
O	-0.510821	1.663970	1.491076
H	0.337892	2.066445	1.756188
O	3.920387	1.773738	2.929779
O	1.934059	2.378584	2.184370
H	4.017846	2.725740	2.959560

FTS1b

H	0.172443	0.132711	0.289237
S	0.063925	-0.116466	1.595613
S	2.094564	0.037894	2.319637
C	2.116412	1.797664	2.518069
O	0.656623	-1.862931	1.294607
H	-0.097656	-2.401512	1.523348
O	3.263897	2.144121	3.092848
O	1.275604	2.567074	2.190043
H	3.279465	3.097474	3.173564

CPFTS1b

H	0.624279	0.243807	0.496441
S	0.191840	-0.328376	1.619371
S	2.818940	0.064514	2.724763
C	2.290370	1.721639	2.602299
O	0.107355	-1.880710	1.085240
H	-0.791249	-2.085770	0.847399
O	3.191244	2.566355	3.091177
O	1.249304	2.088150	2.135220
H	2.844658	3.452705	2.990871

CRBTS2a = CRFTS2b

S	0.319824	0.651392	-0.114438
S	-0.005214	0.173615	1.843167
C	1.993341	0.077341	-0.378129
H	0.447368	1.310950	2.373694
O	-0.343174	-2.027600	-0.658034
H	-0.964139	-1.736717	-1.330610

O	2.261985	0.215115	-1.671972
O	2.741431	-0.328711	0.437130
H	3.156676	-0.086107	-1.826751

BTS2a

S	0.175676	0.134377	0.007408
S	0.400156	0.392105	2.093895
C	1.936562	-0.073061	-0.287381
H	-0.824552	0.912874	2.183164
O	-0.111822	-1.353966	-1.421270
H	-0.957142	-1.711560	-1.153200
O	2.198226	0.050242	-1.569150
O	2.727290	-0.262955	0.569892
H	3.130171	-0.119910	-1.704252

CPBTS2a = CPFTS2b

S	0.480723	0.994991	-1.572841
S	-0.147411	-1.000117	2.795238
C	2.067776	0.395825	-1.106389
H	-0.244748	-0.427558	1.591861
O	-0.556794	0.119656	-0.660617
H	-0.761456	-0.703151	-1.095605
O	2.041818	-0.616392	-0.253209
O	3.045986	0.891309	-1.559775
H	2.947218	-0.857514	-0.056519

CRFTS2a

C	0.104792	-0.032555	-0.099305
S	-0.162440	-0.014120	1.669058
S	1.738344	-0.082869	2.406942
H	1.975667	1.228870	2.345316
O	0.137914	2.744338	1.485521
H	-0.708835	2.908713	1.907814
O	-1.089724	-0.008505	-0.681954
O	1.139561	-0.062195	-0.662601
H	-0.961083	-0.002924	-1.629915

FTS2a

C	0.038700	0.156645	-0.141925
S	-0.243263	0.414557	1.588500
S	1.642913	-0.068233	2.502896
H	2.306418	1.008495	2.081568
O	0.259063	2.118103	1.757593
H	-0.517424	2.628572	1.532500
O	-1.060798	-0.372208	-0.678917
O	1.038118	0.406395	-0.723990
H	-0.888699	-0.532122	-1.606117

CPFTS2a

C	-0.410064	0.199285	-0.077072
S	-0.884636	1.789917	0.503855
S	2.901470	1.077789	2.110676
H	2.217957	0.036050	1.621455
O	-0.362510	1.726988	2.032870
H	0.593421	1.820529	2.071171
O	-0.902948	0.017194	-1.296876
O	0.265935	-0.586532	0.504760
H	-0.607629	-0.833036	-1.620114

FTS2b

C	0.087487	-0.153252	-0.152719
S	0.022883	-0.260161	1.623471
S	2.012484	0.082578	2.304847
H	1.869506	1.406384	2.242565
O	0.532977	-1.982044	1.809310
H	-0.282803	-2.475088	1.874858
O	-1.103516	0.264083	-0.584135
O	1.024319	-0.380709	-0.834626
H	-1.056623	0.359409	-1.534843

HTS3b

C	0.027252	0.185773	0.129448
S	0.097658	-0.345817	1.824146
S	2.030471	0.063927	2.311121
H	1.925023	1.478389	2.352278
O	0.828582	0.858265	-0.432796
O	-1.106384	-0.239581	-0.404969
H	-1.176560	0.110497	-1.292936
O	1.887310	2.706750	1.646497
H	1.715260	2.392515	0.750267

CPHTS3a = CPHTS3ab

C	-0.805125	-0.306581	-0.898172
S	-0.470755	-1.607337	0.310475
S	0.881828	-0.836409	1.491958
H	2.000197	2.673451	0.701961
O	-0.302946	0.760119	-0.939135
O	-1.718828	-0.762054	-1.736511
H	-1.910969	-0.085940	-2.387213
O	1.521733	2.964627	-0.063414
H	0.957837	2.235274	-0.304298

HTS3a

C	0.068626	-0.003906	0.065518
S	0.158948	0.099769	1.848911
S	2.083922	-0.420017	2.216143
H	2.685680	0.817506	1.994891
O	0.948278	-0.256319	-0.678099
O	-1.184460	0.263940	-0.286202
H	-1.245688	0.221642	-1.240063
O	3.272508	2.156048	2.321419
H	3.022330	2.283890	3.239806

CRPTS12a = CRPTS12b

C	-0.389628	-0.026706	-0.485775
S	-0.499791	0.109334	1.285527
S	1.455231	-0.011544	1.864784
H	1.760572	1.282172	1.755576
O	0.613359	-0.076428	-1.126073
O	-1.611485	-0.051095	-0.974593
H	-1.568506	-0.111728	-1.939776
O	-0.643882	-0.233466	-3.626760
H	0.153621	-0.214280	-3.072677

PTS12a

C	-0.028506	-0.032835	0.003034
S	-0.022118	0.061202	1.779492
S	1.957582	-0.003018	2.294480
H	2.215702	1.302238	2.200440
O	1.022286	-0.038971	-0.647798
O	-1.168425	-0.084141	-0.507902
H	-0.795152	-0.105219	-1.677254
O	-0.007357	-0.037170	-2.536863
H	0.394899	-0.891440	-2.690508

CPPTS12a = CPPTS12b

C	-0.167854	-0.048916	-0.307662
S	-0.623266	0.310019	1.361897
S	1.200416	0.141082	2.307521
H	1.596364	1.406300	2.157774
O	1.109047	-0.247672	-0.495030
O	-0.950339	-0.101129	-1.202206
H	-0.803020	-0.330797	-3.214254
O	-0.692906	-0.418296	-4.157253
H	-1.568599	-0.493118	-4.513924

PTS12b

C	-0.179529	-0.016024	0.040256
S	0.012072	-0.016043	1.808978
S	2.035746	0.019059	2.112357
H	2.201204	1.342570	2.100896
O	0.792619	0.085878	-0.716184

O	-1.363583	-0.109373	-0.350139
H	-1.114813	-0.093071	-1.552276
O	-0.415409	-0.111189	-2.487188
H	-0.128279	0.774065	-2.708235

CRHTS5a

H	-1.572972	1.149711	-0.516093
S	-0.975313	2.190279	-1.103995
O	0.580721	1.833855	-0.659414
H	0.750768	2.221715	0.192338
S	1.397276	-1.087061	-0.402675
C	-0.054539	-1.536440	0.459442
O	-0.019724	-2.799616	0.860584
O	-0.963047	-0.794124	0.660609
H	-0.837540	-2.990039	1.320787

HTS5a

H	-0.487938	-0.511714	0.960527
S	0.350193	0.381705	1.504927
O	1.726885	-0.161616	0.982973
H	2.132252	-0.991749	1.504222
S	2.783498	-2.385949	2.385199
C	1.232760	-3.178365	2.425640
O	1.282975	-4.365479	3.015993
O	0.223274	-2.715603	1.979242
H	0.400931	-4.736769	3.006914

CPHTS5a

H	-1.635747	1.117126	-0.434729
S	-1.147168	2.296854	-0.882159
O	0.333835	2.084543	-0.840460
H	1.191569	0.263527	-0.192394
S	1.579849	-0.940404	0.240133
C	-0.058264	-1.514536	0.494762
O	-0.038349	-2.760272	0.952906
O	-1.063238	-0.904623	0.296694
H	-0.942788	-3.043181	1.080706

CRHTS6a

H	-1.302402	0.984275	-0.438502
O	-1.593558	1.807346	-0.020820
S	-0.643668	2.161522	1.217766
H	0.869256	0.057687	0.904170
S	1.410939	-1.085215	0.458112
C	0.249468	-1.265458	-0.837668
O	0.496138	-2.361287	-1.533129
O	-0.655357	-0.524370	-1.092644
H	-0.154738	-2.429435	-2.231231

HTS6a

H	0.720922	-1.180757	-0.154000
O	0.417582	-0.194471	0.388402
S	1.324515	0.159600	1.586459
H	2.252073	-1.084353	1.439955
S	3.027039	-2.578304	0.929899
C	1.981226	-2.887470	-0.366521
O	2.224160	-3.978031	-1.058197
O	1.010061	-2.200303	-0.738555
H	1.575193	-4.046531	-1.757919

CPHTS6a

H	-0.890574	0.178913	-0.727146
O	-1.293658	1.614146	0.100347
S	-0.576115	2.176162	1.290017
H	0.408564	1.261399	1.481184
S	1.258124	-0.952318	0.427692
C	0.283339	-1.312895	-0.841627
O	0.472764	-2.386221	-1.569987
O	-0.737586	-0.623195	-1.260603
H	-0.188503	-2.429520	-2.259389

CRHTS8a = CRHTS8b

C	-0.537371	0.509989	-0.974187
S	-0.991980	1.226474	0.566145
O	0.382024	1.057085	1.401550
H	0.503255	0.144228	1.677328
S	1.271766	-2.149089	1.509654
H	1.340238	-1.677981	0.258748
O	-1.518646	0.700793	-1.848663
O	0.469843	-0.078107	-1.203681
H	-1.280429	0.273942	-2.670607

HTS8a

C	0.052734	0.015900	-0.108582
S	-0.099145	-0.024551	1.674057
O	1.392636	0.008164	2.106415
H	1.933319	-1.016212	2.070031
S	2.602081	-2.471345	2.121084
H	2.342420	-2.633519	3.418791
O	-1.163053	0.092548	-0.629914
O	1.071437	-0.030165	-0.698643
H	-1.094475	0.097995	-1.584600

CPHTS8a = CPHTS8b

C	-0.832385	0.602794	-1.026577
S	-1.075756	1.461647	0.555973
O	-0.129274	0.792017	1.475322
H	1.485080	-1.414465	0.213665
S	2.335663	-2.010672	1.047525
H	1.973479	-1.238471	2.068895
O	-1.644195	1.136121	-1.923445
O	-0.070934	-0.279536	-1.197420
H	-1.527425	0.693138	-2.764641

HTS8b

C	-0.023964	0.000381	0.019467
O	-0.043389	0.095845	1.194661
O	1.051568	-0.065685	-0.750960
H	1.834048	-0.032633	-0.200742
S	-1.475294	-0.107664	-1.019584
O	-2.605609	0.133144	0.017792
H	-2.944307	-0.815493	0.599303
S	-3.302892	-2.126479	1.436350
H	-2.396732	-1.846488	2.373464

QCISD/6-311+G(2df,2p) optimized geometries

HSSCOOH

C	0.000958	0.004869	0.016767
S	-0.004999	-0.026089	1.808932
S	2.010777	-0.012904	2.218826
H	2.187132	1.316114	2.173233
O	0.943987	0.114699	-0.706312
O	-1.276805	-0.103573	-0.388598
H	-1.270166	-0.067314	-1.352486

OHSCOOH

C	-0.003543	0.002556	0.017383
S	-0.008106	-0.008767	1.790411
O	1.614127	0.003875	2.059369
H	1.969231	-0.859938	1.832198
O	0.962891	-0.123105	-0.677105
O	-1.266432	0.140806	-0.419650
H	-1.240093	0.098164	-1.382697

SCOOH

S	0.017743	0.000103	0.013112
C	-0.008254	-0.000634	1.767818

O	0.997712	0.000327	2.423931
O	-1.251320	-0.002421	2.264902
H	-1.170522	-0.002732	3.227110

HSSCO2

C	0.037179	0.011789	0.033095
S	-0.046992	0.048626	1.813583
S	1.969396	-0.032785	2.231236
H	2.215678	1.282172	2.128538
O	1.074926	0.085225	-0.627268
O	-1.059683	-0.076860	-0.601493

SSCOOH

C	-0.001957	-0.000008	0.000925
O	-0.004555	-0.000012	1.190653
O	1.083830	0.000000	-0.787289
H	1.858229	0.000003	-0.211196
S	-1.455699	-0.000018	-1.091511
S	-2.973392	-0.000047	0.167187

CRBTS1a

S	0.169527	-0.357998	0.683359
S	0.744393	-0.580293	2.655631
C	1.650039	0.081396	-0.208368
H	0.478845	0.671898	3.056231
O	-2.078679	-0.236301	3.185874
H	-2.073258	-1.161713	3.471700
O	1.602936	0.203899	-1.400295
O	2.744015	0.259318	0.538459
H	3.452738	0.491566	-0.074134

BTS1a

S	0.086180	-0.226539	0.133397
S	0.019738	-0.185408	2.234849
C	1.806897	-0.008387	-0.286145
H	-0.435886	1.066099	2.329817
O	-1.399871	-0.449660	3.857291
H	-1.418149	-1.415175	3.900885
O	2.146881	-0.028315	-1.434734
O	2.626275	0.169208	0.755221
H	3.513344	0.271014	0.388229

CPBTS1a

S	0.010962	0.274059	-0.142301
S	-0.280477	0.233547	2.205594
C	1.765551	0.062977	-0.221984
H	-1.556985	0.487925	1.911264
O	-0.794759	-0.643903	3.593235
H	0.006614	-0.889643	4.066191
O	2.398685	0.239256	-1.225034
O	2.321996	-0.323155	0.946428
H	3.269198	-0.393159	0.775420

CRBTS1b = CRFTS1b

S	-0.667313	0.807995	-0.438139
S	-0.398592	0.173216	1.502135
H	0.627779	0.959245	-0.751950
C	-0.454875	1.737188	2.375410
O	0.494960	-1.765503	-1.061764
H	-0.362603	-1.971811	-1.461725
O	-0.385009	1.459652	3.689508
O	-0.529149	2.832940	1.908089
H	-0.397227	2.303583	4.156527

BTS1b

S	-0.093676	0.129062	-0.049010
S	-0.131975	0.038305	2.046383
H	1.235202	0.066231	-0.158499
C	-0.495205	1.752282	2.422681
O	0.048089	-1.184878	-1.765925
H	-0.880689	-1.440202	-1.847311
O	-0.624697	1.852200	3.756437

O	-0.607320	2.656529	1.651430
H	-0.814016	2.777993	3.951951

CPBTS1b

S	0.406487	-0.006912	-0.033152
S	0.474086	0.097718	2.311408
H	1.073427	-1.156286	0.101577
C	-0.513592	1.568931	2.316061
O	-0.383170	-0.643614	-1.420831
H	-0.961659	0.057972	-1.737745
O	-0.564552	2.085986	3.555805
O	-1.073583	2.059402	1.370873
H	-1.117746	2.874755	3.499180

CRFTS1a = CRHTS3a = CRHTS3b

H	0.311306	0.138465	0.423693
S	0.301020	-0.294133	1.693868
S	2.333182	-0.231797	2.015253
C	2.572462	1.473620	2.486689
O	-0.589761	2.735770	0.748452
H	0.133012	2.692927	1.398584
O	3.849725	1.620686	2.859322
O	1.764802	2.360405	2.471931
H	3.977748	2.550306	3.084573

FTS1a

H	-0.314676	-0.267548	0.375745
S	0.052653	0.116434	1.616833
S	2.239680	0.118990	1.635303
C	2.566429	1.612763	2.538198
O	0.039634	1.775679	0.810020
H	0.246726	2.371051	1.542667
O	3.889238	1.722507	2.727942
O	1.760302	2.403244	2.952240
H	4.032448	2.528552	3.239820

CPFTS1a

H	0.282096	0.122067	0.027542
S	-0.262308	0.071505	1.260264
S	2.379918	-0.218437	2.467262
C	2.705233	1.498281	2.489240
O	-0.555421	1.659551	1.506513
H	0.296758	2.062521	1.769147
O	3.940093	1.763166	2.930436
O	1.941347	2.385339	2.159438
H	4.034932	2.724181	2.927973

FTS1b

H	0.191008	0.163578	0.306592
S	0.067074	-0.117973	1.613184
S	2.109279	0.016088	2.338259
C	2.117310	1.787735	2.515030
O	0.661411	-1.878575	1.284044
H	-0.118501	-2.396644	1.513633
O	3.270048	2.150972	3.102305
O	1.266285	2.556532	2.164742
H	3.261363	3.114315	3.159178

CPFTS1b

H	0.627262	0.246925	0.513117
S	0.174279	-0.333462	1.633836
S	2.815141	0.057193	2.732730
C	2.284879	1.727066	2.603401
O	0.114119	-1.904634	1.084771
H	-0.789720	-2.085266	0.816853
O	3.212564	2.569204	3.086622
O	1.233022	2.105954	2.142370
H	2.855195	3.459334	2.979082

CRBTS2a = CRFTS2b

S	0.289532	0.730070	-0.098601
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S	-0.033431	0.204358	1.862671
C	1.934191	0.061589	-0.378579
H	0.487776	1.312716	2.410935
O	-0.229194	-1.987001	-0.646231
H	-0.797964	-1.720135	-1.383722
O	2.198510	0.200247	-1.689177
O	2.675327	-0.397916	0.432982
H	3.083351	-0.154649	-1.836220

BTS2a

S	0.163449	0.196539	0.001174
S	0.344805	0.305997	2.099272
C	1.921751	-0.074665	-0.285232
H	-0.766826	1.053450	2.182767
O	-0.099989	-1.405559	-1.463765
H	-0.910862	-1.790380	-1.104941
O	2.196905	0.154641	-1.566455
O	2.701936	-0.394185	0.560381
H	3.123395	-0.077692	-1.704093

CPBTS2a = CPFTS2b

S	0.429143	1.057983	-1.397130
S	0.224918	-0.626430	2.738112
C	2.009742	0.399198	-0.951235
H	-0.234855	-0.420308	1.492484
O	-0.641618	-0.021620	-0.742963
H	-0.744187	-0.757189	-1.352656
O	1.952914	-0.794398	-0.345993
O	3.012586	1.002848	-1.210619
H	2.864468	-1.043036	-0.147857

CRFTS2a

C	0.101135	0.005238	-0.051737
S	-0.163240	-0.050311	1.725064
S	1.767343	-0.105339	2.427044
H	1.980041	1.217806	2.350811
O	0.143103	2.638220	1.364083
H	-0.717954	2.827743	1.765074
O	-1.111981	0.041079	-0.629694
O	1.143697	0.010318	-0.627677
H	-0.967950	0.093999	-1.582091

FTS2a

C	0.031704	0.172435	-0.126578
S	-0.273791	0.414332	1.615269
S	1.637616	-0.078271	2.520856
H	2.293827	0.974081	2.009088
O	0.270489	2.126687	1.771741
H	-0.509538	2.631461	1.509225
O	-1.057032	-0.399003	-0.675121
O	1.037157	0.460652	-0.704683
H	-0.855404	-0.542171	-1.607689

CPFTS2a

C	-0.405983	0.196273	-0.063078
S	-0.831988	1.821395	0.493486
S	2.881633	1.110492	2.027919
H	2.189073	0.041749	1.590874
O	-0.379886	1.719456	2.063146
H	0.584706	1.791197	2.111455
O	-0.858378	0.035558	-1.317265
O	0.209655	-0.628728	0.554864
H	-0.577835	-0.839209	-1.610676

FTS2b

C	0.078275	-0.166107	-0.149967
S	0.009552	-0.258391	1.640118
S	2.017978	0.089509	2.313792
H	1.857833	1.419850	2.245305
O	0.555939	-1.989334	1.787392
H	-0.273423	-2.473981	1.875571

O	-1.110626	0.297316	-0.583724
O	1.016058	-0.433450	-0.836583
H	-1.044871	0.375787	-1.543175

HTS3b

C	0.030474	0.190183	0.132398
S	0.089762	-0.335733	1.838661
S	2.046479	0.061906	2.304065
H	1.921578	1.467428	2.380402
O	0.849277	0.849441	-0.446555
O	-1.124126	-0.228356	-0.399431
H	-1.173005	0.127818	-1.295117
O	1.881086	2.719879	1.627959
H	1.707088	2.358150	0.740676

HTS3a

C	0.092479	0.005165	0.091206
S	0.136795	0.163956	1.880210
S	2.044668	-0.450152	2.287417
H	2.693038	0.741437	1.979943
O	0.988522	-0.312320	-0.628156
O	-1.151178	0.323819	-0.305698
H	-1.167744	0.253274	-1.267784
O	3.278330	2.131905	2.285787
H	2.895233	2.305469	3.159400

CRPTS12a = CRPTS12b

C	-0.389492	-0.026241	-0.472121
S	-0.514495	0.111047	1.307078
S	1.459139	-0.017027	1.872788
H	1.761953	1.282691	1.735742
O	0.626491	-0.071820	-1.114638
O	-1.624610	-0.054786	-0.968973
H	-1.559232	-0.111587	-1.939401
O	-0.646142	-0.233167	-3.649317
H	0.155879	-0.212851	-3.090927

CPPTS12a = CPPTS12b

C	-0.162564	-0.017405	-0.240925
S	-0.666181	0.333488	1.424186
S	1.192786	0.092684	2.299881
H	1.635864	1.344079	2.101611
O	1.090029	-0.219563	-0.460516
O	-0.941055	-0.061708	-1.179703
H	-0.794476	-0.218609	-3.279144
O	-0.727770	-0.289830	-4.233421
H	-1.526790	-0.745663	-4.495105

PTS12a

C	-0.039701	-0.033241	0.009605
S	-0.034045	0.053877	1.794296
S	1.967205	-0.013619	2.283388
H	2.217059	1.299438	2.167528
O	1.027852	-0.030398	-0.642715
O	-1.189849	-0.086592	-0.505764
H	-0.787369	-0.101935	-1.698282
O	-0.008959	-0.026732	-2.548890
H	0.416718	-0.890152	-2.642044

PTS12b

C	-0.190289	-0.018946	0.048270
S	-0.000639	-0.012849	1.825144
S	2.041490	0.015708	2.102760
H	2.201881	1.347085	2.061629
O	0.799060	0.087632	-0.709908
O	-1.384097	-0.118363	-0.346919
H	-1.107483	-0.097075	-1.574748
O	-0.414933	-0.114695	-2.499230
H	-0.104962	0.787375	-2.658533

Reactions starting by HSSCN + OH

BH&HLYP/6-311+G(2df,2p) optimized geometries

HSSCN

C	-0.004531	-0.004612	0.001096
S	-0.016649	-0.022258	1.693111
S	1.993058	0.019031	2.149325
H	2.140990	1.345121	2.150470
N	-0.058528	0.010539	-1.138019

SCN

S	0.253056	0.478988	1.093518
C	-0.129062	-0.513575	2.321593
N	-0.401489	-1.221145	3.197032

SH

S	0.011863	-0.020785	0.004435
H	-0.105534	-0.168441	1.325552

HSCN

N	-1.848235	0.594475	-0.435514
C	-1.412728	1.617891	-0.683014
S	-0.681891	3.099364	-1.034682
H	-1.824794	3.740576	-1.283550

OSCN

C	-0.753775	0.838598	-0.779350
S	-0.666742	1.360858	0.861197
O	0.724179	1.790257	1.094779
N	-0.882774	0.478123	-1.853706

CRFTS1a = CRBTS1b

H	0.241871	0.236814	0.260323
S	-0.038157	0.183964	1.563283
S	1.907651	0.146352	2.253311
C	2.201646	1.795113	2.503914
O	0.770901	-2.464553	1.194551
H	-0.001480	-2.817530	1.643615
N	2.461575	2.889646	2.691838

FTS1a

H	0.157486	0.102463	0.203272
S	0.047674	-0.056026	1.523547
S	2.101201	0.041890	2.202650
C	2.159849	1.703228	2.485647
O	0.615291	-1.849519	1.282204
H	-0.088137	-2.367146	1.667985
N	2.233915	2.824545	2.684862

CPFTS1a = CPFTS1b = CPBTS1b = CPBTS1a

H	0.068720	0.164802	0.264177
S	-0.243303	-0.341902	1.462021
S	2.551506	0.235923	2.509893
C	2.379535	1.869879	2.568088
O	0.312602	-1.869495	1.242314
H	-0.401317	-2.426755	0.948246
N	2.251853	3.013760	2.601370

CRFTS1b = CRBTS1a = CRHTS3b = CRHTS3a

H	-0.036872	0.027371	0.728618
S	0.526544	-0.785625	1.626052
S	2.436976	-0.022995	1.478720
C	2.307267	1.386523	2.403734
O	-0.278475	2.660641	0.983795
H	0.365987	2.971875	1.631296
N	2.226936	2.366865	2.982846

FTS1b

H	0.160280	0.079558	0.063013
S	0.009610	0.029528	1.390353
S	2.013703	-0.073439	2.193130
C	2.616544	1.489604	2.368943
O	0.090714	1.871777	1.272697
H	-0.380000	2.196372	2.038007
N	3.092793	2.515030	2.527127

BTS1b

S	-0.114094	-0.048978	-0.045261
S	-0.141987	0.002301	2.071064
H	1.198103	0.115727	-0.156902
C	-0.735765	1.558254	2.333920
O	0.198731	-1.293594	-1.757360
H	-0.650606	-1.724121	-1.863642
N	-1.138753	2.602113	2.558620

BTS1a

S	-0.091986	-0.118634	-0.041784
S	-0.291148	-0.084075	2.054675
C	-0.710335	1.525629	2.338520
N	-0.993070	2.603766	2.581297
H	1.099183	0.467459	-0.082652
O	-0.309906	0.886488	-1.947064
H	-1.258828	0.956701	-2.060579

CRFTS2a = CRBTS2b

C	0.113099	-0.054068	1.146330
S	0.346831	1.595320	1.438551
S	1.985230	1.583312	2.689168
H	2.921593	1.611937	1.738899
O	-0.572361	-4.071135	0.438760
H	-0.411810	-3.128867	0.585232
N	-0.086424	-1.151848	0.917079

FTS2a

C	0.053364	-0.024989	0.016894
S	0.018124	-0.164740	1.687630
S	2.044268	-0.009742	2.354804
H	2.013014	1.322424	2.308091
O	0.398298	-1.949362	1.836435
H	-0.449247	-2.390117	1.793455
N	0.023070	0.142610	-1.114603

CPFTS2a = CPFTS2b

C	-0.767866	-0.356513	-0.536538
S	-0.010206	-0.007980	0.935669
S	2.084587	0.650546	4.019920
H	2.993566	0.675504	3.042702
O	0.826685	-1.388035	1.189571
H	0.275212	-2.016313	1.648095
N	-1.306271	-0.543780	-1.525502

FTS2b

C	0.070787	-0.032819	-0.101551
S	-0.153883	0.195067	1.543022
S	1.796662	0.025495	2.476159
H	2.186143	1.287551	2.297645
O	0.118375	1.970290	1.624206
H	-0.720711	2.362460	1.384800
N	0.179002	-0.259782	-1.218282

BTS2b

S	0.089017	-0.103719	0.001382
S	0.027138	0.021038	2.130521
C	1.766190	-0.018682	-0.176647
H	-0.711463	1.131211	2.131765
O	0.060641	-1.254792	-1.655154
H	-0.866927	-1.468736	-1.758950
N	2.894669	0.062129	-0.304011

CPBTS2b = CPBTS2a

S	-0.653935	0.116526	1.723396
S	1.068513	0.697627	2.694844
C	-0.052666	-0.458371	0.250815
H	1.116313	1.943755	2.219896
O	1.243784	-1.891687	-3.407057
H	0.935930	-1.556379	-2.553874
N	0.296859	-0.854261	-0.758449

BTS2a

S	-0.046228	0.016718	-0.115110
S	0.135719	0.361101	1.970463
H	1.023929	-0.601275	2.222097
C	-0.875766	-1.459244	-0.054952
N	-1.424999	-2.457028	-0.027661
O	0.740989	-0.416047	-1.947723
H	1.398213	-1.092740	-1.780737

HTS3b

H	0.357368	-0.082268	-0.303829
S	0.271567	-0.141862	1.091141
S	2.266338	-0.322098	1.503853
C	2.534369	-1.985824	1.340671
O	0.393569	0.429163	-1.686989
H	0.495711	1.379509	-1.589189
N	2.778369	-3.095654	1.246318

CPHTS3b = CPHTS3a

H	-0.480671	1.152964	-3.496039
S	-0.392236	0.468595	2.365732
S	-0.427930	0.731237	0.415717
C	0.200071	-0.722436	-0.214053
O	-0.310372	0.682074	-2.689669
H	0.049469	-0.162039	-2.938900
N	0.613228	-1.673445	-0.687300

HTS3a

H	0.378130	0.335522	-0.137061
S	0.118579	-0.142401	1.154286
S	2.055363	-0.253710	1.804207
C	2.491869	-1.830377	1.367838
O	0.606024	0.373514	-1.584145
H	0.736662	-0.546994	-1.828449
N	2.836261	-2.879346	1.081679

CRHTS5a = CRHTS6a

H	-0.088956	2.087227	0.246311
S	-0.012252	1.543842	-0.976241
O	-1.408991	0.749262	-1.019068
H	-1.348090	-0.106067	-0.565198
S	1.841641	-0.476382	0.136793
C	0.393009	-1.242872	0.321370
N	-0.665497	-1.688101	0.396933

HTS5a

H	-0.282214	-0.791605	0.589935
S	0.164674	-0.109381	1.660539
O	1.676783	-0.044417	1.388963
H	2.269145	-1.006686	1.600465
S	2.831380	-2.521316	2.012051
C	1.233644	-2.897191	2.228741
N	0.098217	-3.050338	2.347744

CPHTS5a

H	-1.864788	0.613263	-0.441655
S	-1.308837	1.814645	-0.729324
O	0.155074	1.566566	-0.560336
H	1.647087	0.007093	-0.027054
S	1.697984	-1.281270	0.328336
C	0.021822	-1.464676	0.257077

N -1.107963 -1.614219 0.216215

HTS6a

H -0.230396 -0.387075 0.344180
O 0.160600 -0.076644 1.160624
S 1.726588 0.250871 0.955088
H 2.267953 -1.148465 1.274140
S 2.416849 -2.792429 1.185523
C 1.036951 -2.911268 0.260549
N 0.080488 -2.949533 -0.368359

CPHTS6a

H -1.498984 1.165498 -0.545895
O -1.904051 2.031023 -0.677441
S -1.016950 3.163892 0.036272
H 1.793180 -2.248403 1.039416
S 0.801665 -2.840223 0.370298
C -0.016607 -1.404132 0.036813
N -0.610935 -0.468218 -0.217103

CRHTS8a = CRHTS8b

C -1.143115 0.631281 -0.483314
S -0.124750 1.535630 0.521223
O 1.339502 1.125104 -0.048758
H 1.574066 0.253978 0.289079
S 1.386108 -2.068121 0.877363
H 0.247392 -2.187380 0.187586
N -1.850701 0.006220 -1.125819

HTS8a

C -0.395102 0.358310 0.126170
S 0.449713 0.341140 1.600864
O 1.857487 -0.188310 1.210169
H 1.933276 -1.354279 1.206516
S 2.043647 -2.946182 1.265554
H 2.605466 -2.945519 2.474814
N -1.013622 0.396107 -0.831709

CPHTS8a = CPHTS8b

C -0.756958 0.837049 -0.777370
S -0.667653 1.361764 0.863375
O 0.724132 1.789010 1.090573
H 0.723240 -2.226705 -0.689389
S 0.882210 -2.296216 0.630470
H 2.048024 -1.654539 0.598698
N -0.878634 0.480014 -1.853657

HTS8b

C -0.006750 0.018994 -0.006159
S 0.030038 0.052605 1.693063
O 1.547087 -0.014558 2.022233
H 1.949020 -1.107955 2.132831
S 2.494312 -2.603135 2.228987
H 2.905716 -2.626388 0.960782
N -0.089866 -0.000376 -1.143840

QCISD/6-311+G(2df,2p) optimized geometries

HSSCN

C -0.005662 -0.003663 0.006572
S -0.027758 -0.024718 1.712609
S 1.999341 0.013576 2.147426
H 2.137648 1.348387 2.141237
N -0.049229 0.014238 -1.151861

HOSCN

S 0.004511 -0.012406 -0.189217

C	-0.338130	0.294787	1.452360
N	-0.526587	0.501299	2.578284
O	-1.468009	0.285564	-0.874664
H	-1.528177	1.228502	-1.053219

SCN

S	0.257371	0.490184	1.079669
C	-0.129316	-0.514207	2.322366
N	-0.405550	-1.231710	3.210108

SSCN

S	-0.016645	0.000000	-0.012415
S	-0.010101	0.000000	1.970057
C	1.655087	0.000000	2.390305
N	2.763214	0.000000	2.730477

SH

S	0.012212	-0.020348	0.000518
H	-0.105883	-0.168878	1.329469

RFTS1a = CRBTS1b

H	0.245712	0.227324	0.267208
S	-0.056066	0.211235	1.574448
S	1.897264	0.134866	2.277410
C	2.206346	1.798721	2.504901
O	0.782022	-2.491260	1.175960
H	-0.004596	-2.824616	1.632920
N	2.473324	2.913536	2.677987

FTS1a

H	0.165985	0.110777	0.198621
S	0.053310	-0.052497	1.526393
S	2.110946	0.022596	2.199458
C	2.159531	1.699705	2.485846
O	0.612350	-1.863502	1.261290
H	-0.093924	-2.358175	1.692241
N	2.219082	2.840531	2.686317

CPFTS1a = CPFTS1b = CPBTS1b = CPBTS1a

S	-0.384522	-0.607065	0.669329
S	-0.181304	0.213714	2.565290
H	0.844992	-0.310058	0.228240
C	-0.654727	1.829148	2.285787
O	0.446246	-1.417617	-2.231767
H	-0.203389	-1.693773	-2.896035
N	-0.964120	2.938175	2.149578

CRFTS1b = CRBTS1a = CRHTS3b = CRHTS3a

H	-0.052256	0.044931	0.757667
S	0.529132	-0.788627	1.635470
S	2.446785	-0.021077	1.432602
C	2.322391	1.382391	2.392074
O	-0.293917	2.647849	0.984692
H	0.354114	2.972165	1.632500
N	2.242113	2.367022	3.000054

FTS1b

H	-0.030953	-0.023965	0.124331
S	0.004014	0.030632	1.469848
S	2.114699	-0.082203	2.003079
C	2.575442	1.500235	2.408662
O	0.119533	1.854412	1.136431
H	-0.100423	2.268981	1.979657
N	2.921331	2.560338	2.731262

BT1b

S	-0.190877	-0.019742	-0.051519
S	-0.224769	-0.039882	2.059197
H	1.123891	0.193128	-0.162662
C	-0.713668	1.562945	2.358482
O	0.253390	-1.326681	-1.803836

H	-0.586130	-1.804026	-1.866457
N	-1.046207	2.645961	2.607235

BTS3a

S	-0.071553	-0.193737	-0.005702
S	-0.219999	-0.089934	2.089793
C	-0.724187	1.524214	2.290756
N	-1.066646	2.616537	2.474182
H	1.128727	0.389432	-0.093255
O	-0.322468	0.925060	-1.953240
H	-1.279964	1.065761	-1.960122

CRFTS2a = CRBTS2b

S	-0.673813	0.127267	1.750914
S	1.076175	0.699247	2.707117
C	-0.061509	-0.452115	0.268628
H	1.116174	1.949718	2.221910
O	1.252532	-1.905886	-3.441384
H	0.945091	-1.567705	-2.582474
N	0.300147	-0.853318	-0.755141

FTS2a

C	0.043853	-0.032547	0.017438
S	0.012173	-0.154716	1.708364
S	2.048832	-0.012520	2.372070
H	2.017495	1.327638	2.310553
O	0.412497	-1.957418	1.807117
H	-0.456200	-2.378443	1.800339
N	0.022241	0.134090	-1.133175

CPFTS2a = CPFTS2b

C	-0.763741	-0.353137	-0.508545
S	-0.088789	0.037139	1.008724
S	2.106082	0.738208	4.010963
H	2.802733	0.402011	2.912865
O	0.904549	-1.266255	1.234801
H	0.387294	-1.962088	1.650492
N	-1.252422	-0.582448	-1.535385

FTS2b

C	0.060760	-0.021948	-0.096799
S	-0.165218	0.181963	1.569410
S	1.804181	0.023912	2.507583
H	2.187483	1.287596	2.273832
O	0.128304	1.969730	1.624691
H	-0.721615	2.344735	1.360463
N	0.182482	-0.237724	-1.233182

BTS2b

S	0.049746	-0.091326	0.005536
S	-0.039449	-0.030441	2.127096
C	1.742087	0.004304	-0.164169
H	-0.596377	1.190062	2.166625
O	0.079277	-1.309998	-1.687112
H	-0.865814	-1.489291	-1.792618
N	2.889795	0.095139	-0.286451

CPBTS2b = CPBTS2a

S	-0.319453	-0.488507	-0.757156
S	-0.888036	0.707589	2.566741
C	1.223019	-0.421663	-0.028819
H	0.407129	0.466952	2.831306
O	0.078819	-1.135433	-2.227172
H	0.336771	-0.415564	-2.809835
N	2.257652	-0.356594	0.491576

BTS2a

S	-0.083341	0.047924	-0.081780
S	0.112520	0.340323	2.000515
H	1.081793	-0.567713	2.192778
C	-0.896211	-1.453539	-0.055962

N	-1.435398	-2.478819	-0.052297
O	0.790279	-0.402670	-1.982614
H	1.382216	-1.134022	-1.754261

HTS3b

H	0.329411	-0.112916	-0.283716
S	0.247443	-0.142318	1.109769
S	2.267853	-0.285263	1.488983
C	2.532347	-1.963306	1.323051
O	0.389383	0.416705	-1.698337
H	0.560571	1.361248	-1.559582
N	2.770283	-3.093183	1.221809

CPHTS3b = CPHTS3a

H	-0.478647	1.142737	-3.512506
S	-0.391302	0.458341	2.381673
S	-0.432088	0.750421	0.418859
C	0.198320	-0.716160	-0.216611
O	-0.312435	0.689309	-2.686398
H	0.050375	-0.162314	-2.935222
N	0.617335	-1.685382	-0.694307

HTS3a

H	0.345541	0.363983	-0.104330
S	0.078962	-0.103281	1.188922
S	2.041917	-0.216340	1.810301
C	2.455637	-1.787343	1.287164
O	0.658500	0.290319	-1.563887
H	0.864490	-0.650391	-1.685080
N	2.777842	-2.840740	0.925265

Reactions starting by HSSNO₂ + OH

BH&HLYP/6-311+G(2df,2p) optimized geometries

HSSNO₂

H	0.035665	0.079097	0.026958
S	0.018868	-0.043252	1.356977
S	1.995687	0.025695	1.694136
N	2.348389	1.803314	1.859273
O	1.490772	2.600499	1.679151
O	3.491087	1.998648	2.142232

HOSNO₂

S	-0.001401	0.003526	-0.000091
O	-0.000081	-0.005102	1.600279
H	0.888738	0.000795	1.948279
N	0.264722	1.726840	-0.337537
O	0.509511	2.463838	0.562042
O	0.188124	1.980986	-1.503624

NO₂

N	0.017130	0.000000	0.004656
O	-0.002876	0.000000	1.174918
O	0.853051	0.000000	-0.815004

SNO₂

S	0.016439	0.000651	0.039979
N	-0.002173	-0.002701	1.780711
O	1.063020	0.001009	2.316744
O	-1.078403	-0.006516	2.294141

HSNO₂

N	0.075548	0.088662	-0.044991
S	0.312549	0.579514	1.702225
O	0.946165	0.386103	-0.797651
O	-0.938604	-0.476657	-0.299613

H 0.914632 -0.577786 1.973613

OSNO2

N 0.049658 -0.073759 -0.029591
S 0.333160 -0.600510 1.758317
O 1.004070 0.532052 2.375328
O -0.976692 0.486351 -0.245906
O 0.921315 -0.344628 -0.791683

CRBTS1b

S -0.694353 -0.386965 0.690306
S -0.596039 0.170738 2.616528
H 0.608586 -0.531149 0.447350
N -0.422687 1.979362 2.543044
O -0.318213 2.527528 1.497134
O -0.423009 2.467938 3.632545
O 0.355119 -1.239029 -2.116878
H -0.213202 -1.159568 -2.888843

BTS1b

S -0.078572 0.082131 0.045358
S -0.090406 0.056487 2.132971
H 1.239195 0.168185 -0.072253
N -0.611700 1.735973 2.571661
O -0.800699 2.537422 1.717552
O -0.720377 1.878555 3.750342
O 0.070147 -1.056315 -1.579597
H -0.831266 -1.319556 -1.763063

CPBTS1b

S 0.330500 -0.219367 -0.704882
H -0.522413 0.490293 0.034116
O 1.537023 -0.369725 0.392708
H 2.227866 0.257247 0.200291
S -1.312609 -2.468566 -0.283683
N -2.417092 -1.589891 -1.320545
O -2.123513 -0.477477 -1.686739
O -3.424641 -2.163560 -1.601054

CRBTS1a = CRFTS1b = CRHTS3b = CRHTS3a

S -0.106795 -0.732095 0.560151
S 0.848056 0.098904 2.116540
H 0.773494 -0.432047 -0.400415
N 0.305911 1.831179 2.110410
O -0.360648 2.255682 1.217334
O 0.705943 2.427040 3.059286
O 0.312825 1.603558 -1.598268
H -0.007005 2.113931 -0.845059

BTS1a

S 0.040317 -0.061990 0.100623
S 0.216783 0.027259 2.164790
H 1.337186 0.070125 -0.154918
N 0.485926 1.792687 2.431782
O 0.595971 2.520166 1.496636
O 0.543758 2.077375 3.587256
O -0.363421 0.880412 -1.652914
H -0.298040 1.808674 -1.424163

CPBTS1a

S 0.180466 -0.317784 -0.555900
S 0.176363 0.154560 2.303280
H 1.513050 -0.186350 -0.619301
N 0.308062 1.889007 2.330661
O 0.273095 2.494884 1.277445
O 0.424752 2.402767 3.396185
O -0.280372 1.157221 -0.993802
H -0.152607 1.762640 -0.246004

FTS1b

H 1.188212 0.192050 0.074825

S	0.114041	0.245337	0.893631
S	1.501103	0.336890	2.552172
N	2.636185	1.647219	2.109059
O	-0.473826	1.819316	1.517225
H	-1.103175	2.123503	0.863675
O	3.404247	1.925007	2.978416
O	2.586790	2.108628	1.011661

CPFTS1b

H	0.682499	2.254944	0.433430
S	0.314138	1.015090	0.756196
S	1.616579	1.363275	3.229690
N	3.056146	1.317532	2.233337
O	-1.268204	1.304376	1.066036
H	-1.796965	1.035575	0.320658
O	4.091600	1.356932	2.824101
O	2.940630	1.258146	1.032813

CRFTS1a

H	0.135588	0.181755	0.158686
S	-0.118282	0.165581	1.469446
S	1.776414	0.105426	2.147611
N	2.199470	1.859952	2.339670
O	0.692683	-2.583690	1.202497
H	-0.073559	-2.886967	1.697102
O	3.284364	1.995752	2.819505
O	1.441574	2.704694	1.996479

FTS1a

H	0.042667	0.023151	0.107570
S	-0.032284	-0.097028	1.435941
S	1.999557	-0.027609	2.127747
N	2.155430	1.744478	2.330442
O	0.505390	-1.859770	1.232086
H	-0.126655	-2.368422	1.736330
O	3.197239	2.057678	2.821854
O	1.279842	2.471860	1.976230

CPFTS1a

H	0.411979	0.194969	0.341009
S	0.057575	-0.333529	1.512424
S	2.694844	0.087710	2.402700
N	2.220882	1.772618	2.337928
O	0.017994	-1.909171	1.066765
H	-0.883053	-2.179460	0.916827
O	3.036141	2.550744	2.728869
O	1.130638	2.062724	1.908029

CRBTS2a

S	0.126785	-0.135265	0.687309
S	0.535591	0.565499	2.520709
N	1.764398	-0.271001	-0.088900
H	0.510275	1.872463	2.245404
O	-0.806246	-1.598114	-2.591887
H	0.080191	-1.393874	-2.271040
O	1.705194	-0.757738	-1.185380
O	2.731093	0.106016	0.475371

BTS2a

S	0.118744	0.093285	-0.062634
S	0.175885	0.183627	2.040577
N	1.955174	-0.047896	-0.348009
H	-0.190945	1.466799	2.079520
O	0.038333	-1.103892	-1.557718
H	-0.867587	-1.410586	-1.549287
O	2.299001	0.343129	-1.410112
O	2.613161	-0.493041	0.529101

CPBTS2a = CPBTS2b

S	-0.117977	-0.386206	-0.688152
S	-0.781143	0.660526	3.282869

N	1.618960	-0.399813	-0.318143
H	0.386789	0.362544	2.707159
O	-0.104403	-0.855076	-2.217305
H	0.094193	-0.128784	-2.804203
O	2.399008	-0.587873	-1.192899
O	1.849268	-0.184630	0.839084

CRBTS2b

S	0.109945	-0.521448	0.203801
S	-0.040995	0.331134	2.010599
N	1.844517	-0.242302	-0.277470
H	-0.328398	1.568650	1.595994
O	-0.340314	2.090255	-0.796784
H	-0.571854	1.883688	-1.706325
O	2.073154	-0.692603	-1.360353
O	2.583090	0.323042	0.452558

BTS2b

S	-0.069858	0.043106	-0.011605
S	-0.164594	-0.080680	2.055032
N	1.778459	-0.032019	-0.222831
H	0.208694	1.168746	2.334695
O	-0.168648	1.163698	-1.639830
H	-0.045258	2.065252	-1.343101
O	2.126703	-0.504207	-1.250216
O	2.448640	0.397305	0.658786

HTS3a

S	-0.092140	0.055823	0.078132
S	-0.349812	-0.427938	1.993995
N	1.709490	0.275763	-0.056856
O	2.078067	0.372802	-1.184515
O	2.364328	0.355248	0.934623
H	-0.271305	0.867496	2.550478
O	0.495792	1.998020	3.011676
H	1.388147	1.769038	2.730961

HTS3b

S	0.042273	-0.015012	-0.059549
S	0.043203	0.188690	1.921308
N	1.812157	-0.132415	-0.491816
O	1.965246	-0.315431	-1.660704
O	2.635882	-0.023224	0.350665
H	0.207251	1.571983	2.009312
O	-0.046390	3.039038	2.157930
H	-0.999719	3.126373	2.074186

CPHTS3a = CPHTS3b

S	-0.931541	-0.731389	-0.264812
S	-0.871938	-1.473208	1.487856
N	0.674331	0.192058	-0.478661
O	0.750268	0.711973	-1.546865
O	1.463536	0.192278	0.402684
H	0.367999	2.352004	1.520626
O	-0.499700	2.357427	1.132664
H	-0.637239	3.239221	0.808636

CRHTS5a

H	-1.752262	1.216864	-0.387117
S	-1.141685	2.371958	-0.737553
O	0.311174	2.037362	-0.632268
H	1.133444	0.259045	-0.085361
S	1.579473	-0.949118	0.286297
N	-0.039828	-1.615478	0.483693
O	-0.077253	-2.754681	0.832157
O	-0.983506	-0.908285	0.263582

HTS5a

H	-0.397028	-0.420388	0.679435
S	0.314699	0.388735	1.477339

O	1.778533	-0.027335	1.081365
H	2.125359	-0.898446	1.515451
S	2.800606	-2.418564	2.345975
N	1.265137	-3.229290	2.377323
O	1.233601	-4.337848	2.811193
O	0.313694	-2.613935	1.959010

CPHTS5a

H	-0.755412	3.023945	-2.127448
S	-0.973560	2.988584	-0.808941
O	-0.313342	1.511615	-0.492286
H	-0.978352	0.829223	-0.543498
S	1.486377	-0.643876	0.492816
N	0.140799	-1.722936	0.266715
O	0.345876	-2.865012	0.538663
O	-0.886703	-1.257240	-0.140574

CRHTS6a

N	-1.049559	0.263724	-1.062770
S	-1.151898	0.211984	0.689910
O	0.023822	0.123706	-1.597602
O	-2.083397	0.435857	-1.630323
H	1.425527	-1.253825	-0.044555
S	1.602509	-0.050680	0.503818
O	2.110216	-0.505369	1.985147
H	1.373634	-0.762108	2.533933

HTS6a

N	0.078320	0.108577	0.062880
S	-0.085061	-0.325490	1.761129
O	1.171809	0.091971	-0.427493
O	-0.942514	0.389316	-0.485200
H	1.576214	-0.722012	1.805834
S	3.033440	-0.462687	1.757280
O	3.388799	-0.829065	3.301019
H	3.573534	-0.031894	3.789178

CPHTS6a

N	-1.291001	0.293259	-1.337963
S	-1.932794	-0.384233	0.162770
O	-0.121500	0.537121	-1.401491
O	-2.102657	0.458383	-2.195449
H	-0.738394	-0.384112	0.769101
S	1.843239	0.018181	0.963316
O	2.486767	-0.395160	2.387081
H	3.424793	-0.222928	2.387879

CRHTS8a = CRHTS8b

N	-0.846046	0.277141	-0.892661
S	-0.762146	1.233773	0.599988
O	0.802909	1.246571	0.888309
H	1.087922	0.415841	1.290802
S	1.660902	-1.816141	1.704196
H	1.443233	-2.001222	0.398374
O	-1.945726	0.240212	-1.360985
O	0.137026	-0.263427	-1.296628

HTS8a

N	0.016566	0.010182	-0.049918
S	0.009843	-0.060653	1.754534
O	1.498710	0.002327	2.096383
H	2.015936	-1.047116	2.070262
S	2.678563	-2.502922	2.085521
H	2.545472	-2.649862	3.404435
O	-1.087152	0.069165	-0.502413
O	1.056392	-0.011933	-0.615025

HTS8b

N	0.004874	-0.016164	0.004634
S	0.011173	0.024888	1.809292
O	1.504507	-0.000465	2.132942

H	1.937886	-1.089701	2.195406
S	2.511413	-2.577347	2.194048
H	2.776670	-2.548853	0.887202
O	-1.092295	0.107884	-0.449583
O	1.034596	-0.167459	-0.562012

CPHTS8a = CPHTS8b

N	-0.304138	0.595621	-0.768088
S	-1.282575	0.901560	0.766905
O	-0.476086	1.802133	1.570440
H	1.360253	-2.456814	-0.037111
S	1.333770	-1.931953	1.186065
H	2.279085	-1.038077	0.903613
O	-0.869275	-0.134964	-1.525379
O	0.751003	1.117667	-0.877684

QCISD/6-311+G(2df,2p) optimized geometries

HSSNO2

H	0.039267	0.084671	0.023521
S	0.008833	-0.042807	1.360418
S	2.002947	0.009098	1.697066
N	2.348120	1.802822	1.858633
O	1.474862	2.606730	1.674897
O	3.506439	2.003487	2.144191

HOSNO2

S	0.000353	-0.011582	-0.004072
O	-0.010063	-0.005586	1.616485
H	0.894949	-0.002042	1.943651
N	0.264837	1.729725	-0.339401
O	0.511999	2.474509	0.574074
O	0.187537	1.985860	-1.521388

NO2

N	0.010051	0.000000	0.001670
O	-0.005462	0.000000	1.190618
O	0.862716	0.000000	-0.827717

SNO2

S	0.016604	0.000483	0.029573
N	-0.002174	-0.001902	1.775729
O	1.076807	0.000743	2.324537
O	-1.092354	-0.006880	2.301737

CRBTS1b

S	-0.728743	-0.429677	0.741783
S	-0.578692	0.163138	2.670680
H	0.578703	-0.559117	0.473479
N	-0.419530	1.983805	2.534407
O	-0.345932	2.507439	1.455184
O	-0.393211	2.509448	3.624498
O	0.363685	-1.234651	-2.142983
H	-0.180077	-1.111530	-2.935863

BTS1b

S	-0.138053	0.116378	0.042604
S	-0.161884	0.024938	2.119599
H	1.184237	0.255415	-0.080683
N	-0.593270	1.742998	2.587925
O	-0.718739	2.582167	1.736564
O	-0.712097	1.864189	3.784338
O	0.111418	-1.099015	-1.623986
H	-0.795290	-1.404188	-1.763391

CPBTS1a = CPFTS1b = CPFTS1a

S	0.394959	0.039143	0.017066
S	0.417799	0.185233	2.375256

H	1.159694	-1.043121	0.197265
N	-0.685480	1.601169	2.393076
O	-1.240368	1.942646	1.369525
O	-0.795326	2.123948	3.477584
O	-0.321618	-0.689633	-1.348614
H	-0.935007	-0.040832	-1.710284

CRBTS1a = CRFTS1b = CRHTS3b = CRHTS3a

S	-0.123175	-0.756146	0.582095
S	0.891182	0.097325	2.109592
H	0.731112	-0.440916	-0.406764
N	0.300151	1.828328	2.106857
O	-0.432477	2.227779	1.232720
O	0.739302	2.452767	3.040786
O	0.360599	1.623684	-1.595866
H	0.005087	2.133331	-0.849443

BTS1a

S	0.051080	-0.133660	0.122183
S	0.256072	-0.004838	2.175295
H	1.352317	-0.008901	-0.161707
N	0.464699	1.798297	2.380470
O	0.539673	2.506992	1.407822
O	0.525329	2.121766	3.541790
O	-0.379047	0.969915	-1.631568
H	-0.251644	1.865137	-1.285193

CPBTS1a

S	0.190989	-0.340292	-0.562351
S	0.136497	0.155377	2.315934
H	1.527175	-0.183678	-0.658737
N	0.314642	1.903634	2.347659
O	0.309734	2.518026	1.284046
O	0.431519	2.410473	3.434296
O	-0.301803	1.150225	-1.014513
H	-0.165944	1.743181	-0.253769

FTS1b

H	1.180224	0.216490	0.062648
S	0.108182	0.217911	0.893082
S	1.508350	0.288307	2.557834
N	2.613489	1.644923	2.102525
O	-0.429217	1.836477	1.540097
H	-1.059281	2.138527	0.872685
O	3.359268	1.975102	2.994596
O	2.572563	2.080212	0.977197

CRFTS1a

H	0.150926	0.087849	0.295056
S	-0.165700	0.266657	1.588010
S	1.709056	0.186156	2.350748
N	2.233313	1.945331	2.315666
O	0.678872	-2.720626	1.104393
H	-0.113166	-3.080887	1.531788
O	3.321541	2.081348	2.815067
O	1.523410	2.776674	1.830269

FTS1a

H	0.050939	0.038786	0.110772
S	-0.023181	-0.099395	1.445762
S	2.023243	-0.049755	2.134566
N	2.154446	1.744118	2.329333
O	0.500409	-1.873225	1.215924
H	-0.145314	-2.359934	1.741525
O	3.205687	2.078676	2.824936
O	1.254957	2.465068	1.965382

CRBTS2a

S	0.118189	-0.137789	0.653537
S	0.514719	0.551458	2.512169
N	1.787801	-0.267242	-0.089459

H	0.501312	1.865143	2.231333
O	-0.840872	-1.591881	-2.557447
H	0.061942	-1.390867	-2.260855
O	1.750190	-0.754087	-1.204542
O	2.754000	0.113252	0.506849

BTS2a

S	0.077194	0.124173	-0.085653
S	0.068416	0.141525	2.010173
N	1.935260	-0.020566	-0.337803
H	-0.018866	1.479264	2.112650
O	0.063473	-1.172451	-1.559614
H	-0.867450	-1.431137	-1.568653
O	2.292053	0.368988	-1.415530
O	2.591686	-0.458373	0.565868

CPBTS2a = CPBTS2b

S	0.000188	0.662414	-0.418311
S	-0.193683	0.565325	3.587508
N	1.709878	0.122350	-0.364898
H	0.860579	0.177232	2.850155
O	-0.243921	0.686750	-2.019862
H	0.099970	1.507965	-2.385543
O	2.334984	0.038350	-1.388872
O	2.094691	-0.095292	0.767156

CRBTS2b

S	0.117738	-0.643812	0.296302
S	-0.006295	0.317762	2.069289
N	1.814149	-0.232143	-0.283472
H	-0.401052	1.507150	1.583919
O	-0.227654	2.131570	-0.834957
H	-0.532021	1.942316	-1.735714
O	2.026368	-0.710721	-1.371023
O	2.537912	0.428295	0.397676

BTS2b

S	-0.059327	-0.014394	0.000176
S	-0.149375	-0.075639	2.063593
N	1.792542	-0.061057	-0.222024
H	0.164617	1.209860	2.289218
O	-0.152757	1.213474	-1.669078
H	-0.093556	2.095135	-1.276112
O	2.139479	-0.551485	-1.261169
O	2.472514	0.405308	0.656326

CRFTS10b

N	0.313806	-0.387020	1.205566
S	0.222406	1.375073	1.676559
S	2.096135	1.758398	2.331865
H	2.642225	2.091565	1.150449
O	-0.977086	-3.670806	-0.173177
H	-0.881003	-2.769531	0.176316
O	-0.773509	-0.807216	0.855960
O	1.351231	-0.985504	1.250032

FTS10b

N	0.004738	-0.030775	-0.141658
S	0.035730	-0.040090	1.771113
S	1.971182	0.006577	2.420354
H	2.082502	1.341999	2.322776
O	0.309563	-1.876672	1.483002
H	-0.461489	-2.268759	1.909172
O	-1.122279	0.005698	-0.575958
O	1.047166	0.024947	-0.732249

CPFTS10b

N	-0.372358	0.101547	-0.843560
S	0.474922	-0.332875	2.950886
S	2.392163	-0.362340	2.241193
H	2.321298	0.706892	1.429988

O	-0.422631	-1.133957	1.797930
H	-0.356558	-2.076518	1.973232
O	-0.109735	-0.932200	-1.366667
O	0.264897	1.000084	-0.393393

CRFTS10a

N	0.070765	-0.236176	-0.105075
S	-0.037851	-0.296961	1.730141
S	1.882315	-0.052558	2.310677
H	1.887587	1.291296	2.299508
O	0.119524	2.663373	1.169478
H	-0.816698	2.914581	1.154680
O	-1.023869	-0.327725	-0.605335
O	1.130826	-0.119601	-0.640488

FTS10a

N	0.085634	-0.090628	-0.168513
S	-0.093147	0.210853	1.743849
S	1.811459	-0.045644	2.378983
H	2.082118	1.270352	2.464667
O	-0.034937	1.984053	1.096259
H	-0.625662	2.439227	1.708554
O	-0.988324	-0.190313	-0.705470
O	1.183657	-0.225856	-0.631395

CPFTS10a

N	-0.008262	0.020951	-1.022662
S	0.174554	0.093307	2.893214
S	2.081503	0.460972	2.251016
H	2.267540	1.659903	2.830377
O	-0.806975	0.720923	1.702884
H	-0.955093	1.649511	1.900327
O	0.316619	1.141075	-1.258887
O	0.557378	-0.953656	-0.645328

HTS3b

S	0.012951	-0.000792	-0.047643
S	0.044509	0.159762	1.956088
N	1.795938	-0.109902	-0.483000
O	1.948486	-0.272391	-1.671882
O	2.630495	-0.013239	0.373568
H	0.234108	1.537802	2.045863
O	-0.029745	3.041149	2.165233
H	-0.976838	3.097613	1.963104

CPHTS3b = CPHTS3a

S	-0.913364	-0.744161	-0.287090
S	-0.915082	-1.330446	1.543862
N	0.711351	0.175365	-0.499250
O	0.834229	0.626610	-1.611741
O	1.472070	0.239682	0.427731
H	0.355470	2.296430	1.461674
O	-0.520214	2.323143	1.073499
H	-0.708743	3.253742	0.953444

HTS3a

S	-0.109835	0.057997	0.084113
S	-0.363717	-0.443615	2.015035
N	1.703893	0.299610	-0.027384
O	2.088684	0.399964	-1.166084
O	2.355876	0.389189	0.985999
H	-0.297784	0.858115	2.554080
O	0.541628	1.994096	2.980956
H	1.403822	1.710895	2.631777