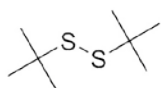
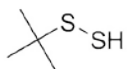


Optimized geometries for species and transition states in “Automatic Mechanism Generation for Pyrolysis of Di-tert-butyl Sulfide”.

Numbers in each row are (X,Y,Z) position of that atom, in Angstroms. Values were computed using B3LYP/6-311G(2d,d,p).

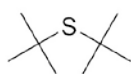


C	0.00000000	0.00000000	0.00000000
C	1.53174626	0.00000000	0.00000000
H	1.92592589	1.01832236	0.00000000
H	1.92493688	-0.52070861	0.87583099
H	1.90251005	-0.51493531	-0.89338576
C	-0.54202927	0.80778440	-1.18969306
H	-0.20123252	0.34900838	-2.12325565
H	-1.63481919	0.82372283	-1.20050709
H	-0.18178776	1.83950922	-1.17167112
C	-0.54374106	-1.42754647	-0.02004175
H	-0.21279405	-1.98530061	0.85749669
H	-1.63521410	-1.44083730	-0.05022088
H	-0.17212111	-1.94947893	-0.90903386
S	-0.63111106	0.98339400	1.48414935
S	0.09609104	0.04223339	3.19259799
C	-1.38458322	-0.74241623	4.06437372
C	-0.74631646	-1.34991877	5.32343573
H	-0.24498389	-0.58860389	5.92644496
H	-1.52702912	-1.80666090	5.93990255
H	-0.01841540	-2.12523500	5.07123423
C	-2.04723653	-1.82552216	3.21483440
H	-2.88218394	-2.26783007	3.76985546
H	-2.44561842	-1.40810813	2.28868822
H	-1.34576804	-2.62387789	2.96389436
C	-2.39271200	0.34729500	4.44180242
H	-3.22320063	-0.09451262	5.00381393
H	-1.92769145	1.11707197	5.06112247
H	-2.80612580	0.82591672	3.55139436



S	0.00000000	0.00000000	0.00000000
H	1.34910281	0.00000000	0.00000000
S	-0.32838525	2.05923063	0.00000000

C	-0.40869231	2.56780253	-1.81069407
C	-0.67837559	4.07854387	-1.72384694
H	0.13115556	4.60320742	-1.21005212
H	-0.75806808	4.48959055	-2.73500045
H	-1.61464630	4.28986572	-1.20097846
C	-1.56056946	1.84866622	-2.51623311
H	-1.62224158	2.18048333	-3.55850056
H	-1.40887513	0.76718250	-2.51795843
H	-2.51502017	2.06155839	-2.03025076
C	0.92680901	2.29269502	-2.50457567
H	0.88578927	2.64280492	-3.54174937
H	1.74864135	2.80740598	-2.00159508
H	1.14833010	1.22318299	-2.52521203



S	0.00000000	0.00000000	0.00000000
C	1.87814002	0.00000000	0.00000000
C	2.20259938	1.50563151	0.00000000
H	1.85449145	1.98717265	0.91606492
H	3.28634454	1.64362073	-0.07354299
H	1.74091962	2.01374297	-0.85058639
C	2.43921604	-0.63514712	-1.28124718
H	3.52706678	-0.50226186	-1.31452201
H	2.23434425	-1.70445158	-1.33420995
H	2.01051579	-0.16401703	-2.16790698
C	2.48910505	-0.64977689	1.24617685
H	2.32937681	-1.72922847	1.26887420
H	3.57233969	-0.48220085	1.24871886
H	2.07766860	-0.21863671	2.16074187
C	-0.73077322	-1.67601539	0.42933793
C	-2.20063625	-1.50848220	0.00080060
H	-2.76223012	-2.40921798	0.26957447
H	-2.66886846	-0.65831191	0.50358086
H	-2.28553145	-1.35737462	-1.07725065
C	-0.67513025	-1.94171716	1.94133548
H	0.34671026	-2.06599466	2.29993434
H	-1.13127698	-1.12000682	2.49688096
H	-1.22473215	-2.86096765	2.17607031
C	-0.10381502	-2.83460196	-0.35362307
H	-0.11948588	-2.64199797	-1.42798578
H	0.92683446	-3.02728341	-0.05051485
H	-0.67422393	-3.75125015	-0.16421380



S	0.00000000	0.00000000	0.00000000
C	1.87105968	0.00000000	0.00000000
H	-0.16002107	1.33513629	0.00000000
C	2.39313028	0.69614930	1.26279000

H	3.48823221	0.65836892	1.28580800
H	2.09529240	1.74757402	1.28963200
H	2.01218154	0.21296246	2.16433100
C	2.27213608	-1.48254056	0.00000000
H	1.89289651	-1.99753010	-0.88606200
H	3.36315531	-1.56723573	-0.00000000
H	1.89289651	-1.99753010	0.88606200
C	2.39313028	0.69614930	-1.26279000
H	3.48823221	0.65836892	-1.28580800
H	2.01218154	0.21296246	-2.16433100
H	2.09529240	1.74757402	-1.28963200

H₂S₂

S	0.00000000	0.00000000	0.00000000
H	1.34788024	0.00000000	0.00000000
S	-0.29725724	2.07647703	0.00000000
H	-0.34188265	2.26304396	-1.33415985

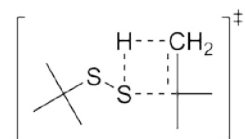
H₂S

S	0.00000000	0.00000000	0.00000000
H	1.34327993	0.00000000	0.00000000
H	-0.06054407	1.34191482	0.00000000



C	-0.00028400	-0.00000400	-0.00010500
H	-0.00131600	-0.00003500	1.08471800
H	0.96837900	0.00002300	-0.48847800
C	-1.13511100	-0.00000100	-0.69953000
C	-1.14823900	0.00001900	-2.20683000
H	-1.67778200	-0.87868600	-2.59328600
H	-1.67799900	0.87859800	-2.59327200
H	-0.13852100	0.00014600	-2.62098000
C	-2.48731800	-0.00001600	-0.03385200
H	-3.07084000	-0.87856300	-0.33307100
H	-2.40315500	-0.00016500	1.05430200
H	-3.07073000	0.87868600	-0.33283400

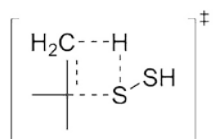
Transition State 1



S	-0.45839400	-0.52516100	0.05632700
C	-3.31620400	0.20533100	0.06623100
C	2.59814500	0.30246600	-0.01958200
C	-3.31554300	1.60687200	-0.45126700
H	-3.01728200	1.65358700	-1.50074400
H	-4.33705000	2.01570600	-0.39294400

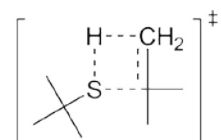
H	-2.66521300	2.25818900	0.13390600
C	-2.91839800	-0.07767400	1.39827600
H	-2.90233300	0.77198500	2.08108700
H	-3.34007200	-0.98214700	1.83778000
H	-1.72556500	-0.38025500	1.33888700
C	-3.90590700	-0.86322400	-0.79539300
H	-3.62736700	-0.74192200	-1.84409300
H	-3.61353700	-1.85995000	-0.46306900
H	-5.00508500	-0.80317700	-0.74684200
S	1.46266800	-1.19260200	-0.19560300
C	4.00358100	-0.27561200	-0.23807100
H	4.10131300	-0.72435100	-1.23005000
H	4.74727900	0.52375500	-0.15465000
H	4.24301900	-1.03762800	0.50821900
C	2.46363300	0.89544600	1.38513200
H	3.13393900	1.75575500	1.49388800
H	1.44153100	1.23448700	1.56745600
H	2.72167700	0.15975600	2.15057400
C	2.26271700	1.34228700	-1.09135400
H	2.93255600	2.20476900	-0.99810800
H	2.37656600	0.92497400	-2.09457800
H	1.23510800	1.69533300	-0.98213800

Transition State 2



S	-0.93890900	0.01391800	0.08119400
C	1.95720000	-0.00005200	0.06361200
C	2.26126100	-1.29890400	-0.60946400
H	1.99787800	-1.28034700	-1.66856200
H	3.34484900	-1.48808000	-0.55119200
H	1.75163300	-2.13480100	-0.12931400
C	1.52886400	0.03079800	1.41395500
H	1.71336000	-0.87262000	1.99510400
H	1.72666800	0.95406300	1.95821600
H	0.28859200	0.03419400	1.37164100
C	2.29104500	1.26373900	-0.66041400
H	2.01953500	1.21203400	-1.71642100
H	1.80919900	2.13172500	-0.20924700
H	3.37984800	1.42487600	-0.61716700
S	-2.99683000	-0.08790200	-0.17264700
H	-3.28995100	1.22921100	-0.21593500

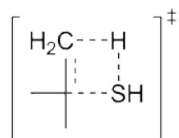
Transition State 3



C	0.00000000	0.00000000	0.00000000
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S	1.86193637	0.00000000	0.00000000
C	4.70275716	0.56102696	0.00000000
C	-0.51872846	-0.52533934	-1.34662509
H	-0.17902407	-1.54887888	-1.52299364
H	-1.61600641	-0.52250200	-1.36483231
H	-0.15790820	0.09436849	-2.17042559
C	-0.45669312	1.45352517	0.20975502
H	-1.55252457	1.50478661	0.21532694
H	-0.09219605	1.84769794	1.16142631
H	-0.09119602	2.10117455	-0.59114951
C	-0.51111361	-0.88297697	1.14812724
H	-1.60833794	-0.88663774	1.16984435
H	-0.17124458	-1.91480953	1.02864212
H	-0.14680723	-0.51856316	2.11103019
C	4.84619430	1.36490255	-1.24787407
H	4.40075761	2.35557321	-1.14987084
H	5.92018475	1.50768131	-1.45011597
H	4.41089803	0.85577207	-2.10776725
C	4.59467114	-0.85661430	-0.06451875
H	4.91736943	-1.31059680	-1.00149556
H	4.92927557	-1.39486080	0.82220031
H	3.40123826	-1.04608974	-0.06733497
C	4.86965159	1.24805200	1.31300879
H	4.41448089	2.23919335	1.31655676
H	4.45922939	0.65842321	2.13271654
H	5.94706450	1.38273441	1.50236674

Transition State 4



S	-1.92623500	-0.00000700	-0.20784200
C	0.98833500	0.00000100	0.12266400
C	1.33771200	-1.28239900	-0.54734700
H	1.21395300	-1.22751900	-1.62905800
H	2.40077700	-1.49509000	-0.34799900
H	0.75405900	-2.11478500	-0.15397400
C	0.46256800	0.00002100	1.44791700
H	0.63332300	-0.91314200	2.01807900
H	0.63342900	0.91316700	2.01807700
H	-0.71572900	0.00009600	1.26811100
C	1.33761300	1.28240900	-0.54738500
H	1.21394400	1.22746700	-1.62910200
H	0.75384100	2.11474700	-0.15408700
H	2.40064200	1.49522300	-0.34796400
H	-3.22584800	-0.00024700	-0.57170500