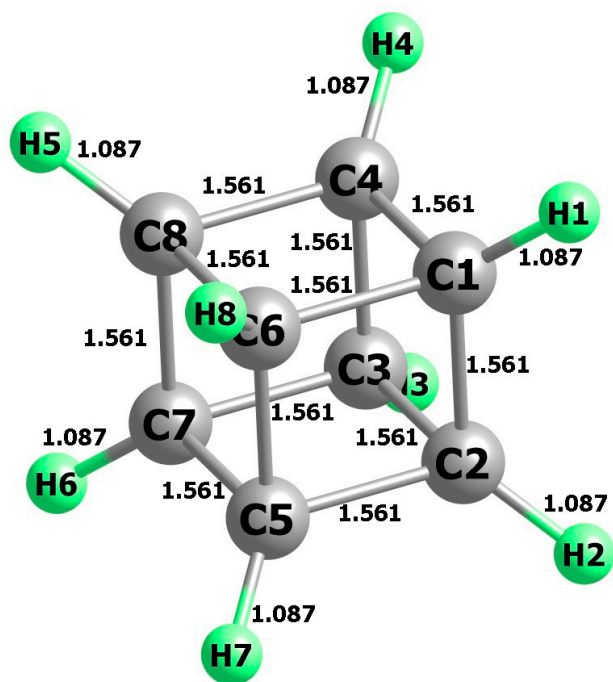


Supplementary Materials

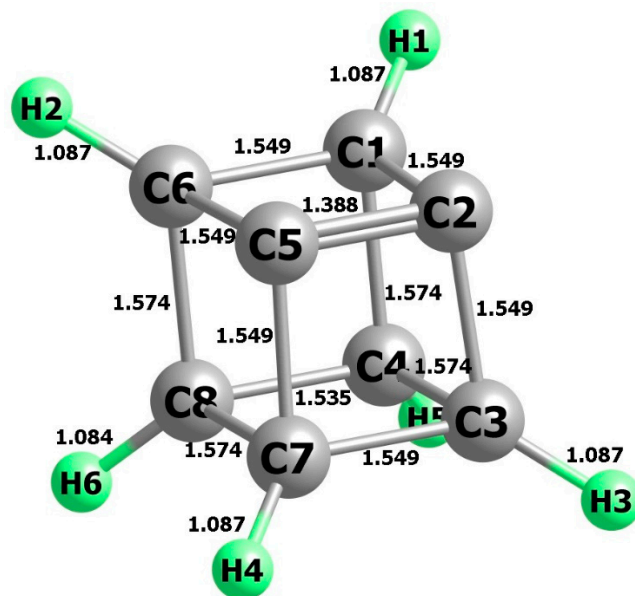
The key geometric paraments of cubane C₈H_n molecular structure

Bond lengths, pm			
(C1C2)	156.1	(C4C8)	156.1
(C1C4)	156.1	(C4H4)	108.7
(C1C6)	156.1	(C5C6)	156.1
(C1H1)	108.7	(C5C7)	156.1
(C2C3)	156.1	(C5H7)	108.7
(C2C5)	156.1	(C6C8)	156.1
(C2H2)	108.7	(C6H8)	108.7
(C3C4)	156.1	(C7C8)	156.1
(C3C7)	156.1	(C7H6)	108.7
(C3H3)	108.7	(C8H5)	108.7
Bond angles, deg			
(C2C1C4)	90.0	(C2C5C6)	90.0
(C2C1C6)	90.0	(C2C5C7)	90.0
(C2C1H1)	125.3	(C2C5H7)	125.3
(C4C1C6)	90.0	(C6C5C7)	90.0
(C4C1H1)	125.3	(C6C5H7)	125.3
(C6C1H1)	125.3	(C7C5H7)	125.3
(C1C2C3)	90.0	(C1C6C5)	90.0
(C1C2C5)	90.0	(C1C6C8)	90.0
(C1C2H2)	125.3	(C1C6H8)	125.3
(C3C2C5)	90.0	(C5C6C8)	90.0
(C3C2H2)	125.3	(C5C6H8)	125.3
(C5C2H2)	125.3	(C8C6H8)	125.3
(C2C3C4)	90.0	(C3C7C5)	90.0
(C2C3C7)	90.0	(C3C7C8)	90.0
(C2C3H3)	125.3	(C3C7H6)	125.3
(C4C3C7)	90.0	(C5C7C8)	90.0
(C4C3H3)	125.3	(C5C7H6)	125.3
(C7C3H3)	125.3	(C8C7H6)	125.3
(C1C4C3)	90.0	(C4C8C6)	90.0
(C1C4C8)	90.0	(C4C8C7)	90.0
(C1C4C12)	125.3	(C4C8H5)	125.3
(C3C4C8)	90.0	(C6C8C7)	90.0
(C3C4H4)	125.3	(C6C8H5)	125.3
(C8C4H4)	125.3	(C7C8H5)	125.3
Selected torsion (dihedral) angles, deg			
(C4C1C2C3)	0.0	(C2C3C7C5)	0.0
(C4C1C2C5)	-90.0	(C2C3C7C8)	90.0
(C4C1C2H2)	135.0	(C2C3C7H6)	-135.0
(C6C1C2C3)	90.0	(C4C3C7C5)	-90.0
(C6C1C2C5)	0.0	(C4C3C7C8)	0.0
(C6C1C2H2)	-135.0	(C4C3C7H6)	135.0
(H1C1C2C3)	-135.0	(H3C3C7C5)	135.0
(H1C1C2C5)	135.0	(H3C3C7C8)	-135.0
(H1C1C2H2)	0.0	(H3C3C7H6)	0.0
(C2C1C4C3)	0.0	(C1C4C8C6)	0.0
(C2C1C4C8)	90.0	(C1C4C8C7)	-90.0
(C2C1C4H4)	-135.0	(C1C4C8H5)	135.0
(C6C1C4C3)	-90.0	(C3C4C8C6)	90.0
(C6C1C4C8)	0.0	(C3C4C8C7)	0.0

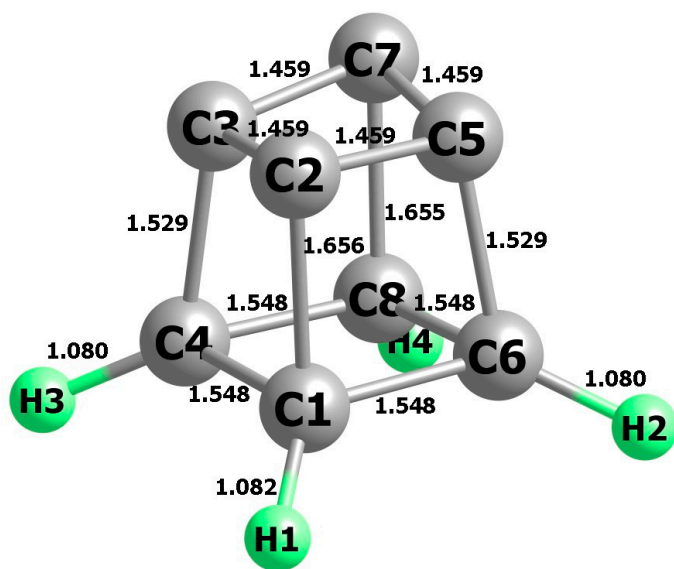
The images of intermediate C_8H_n ($n = 8, 6, 4, 2$) molecular structures of the cubane dehydrogenation reaction



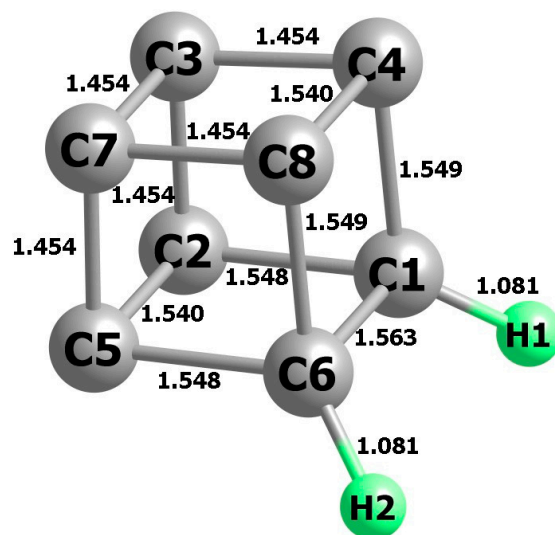
C_8H_8



C_8H_6

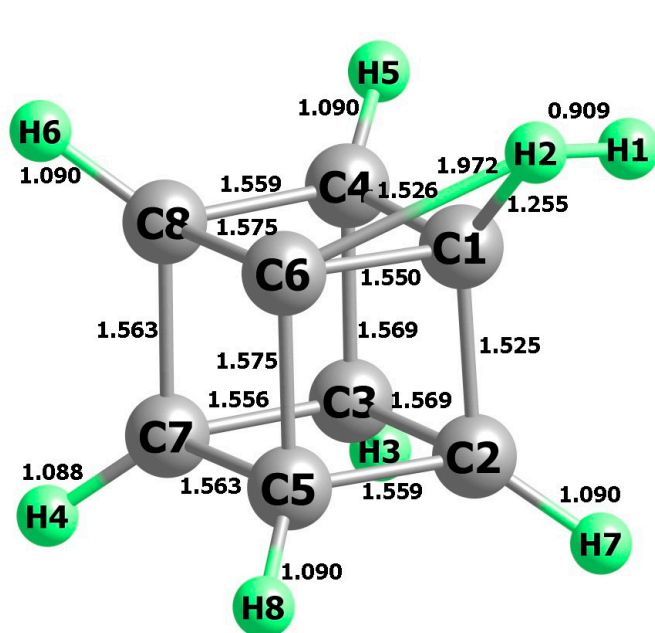


C_8H_4

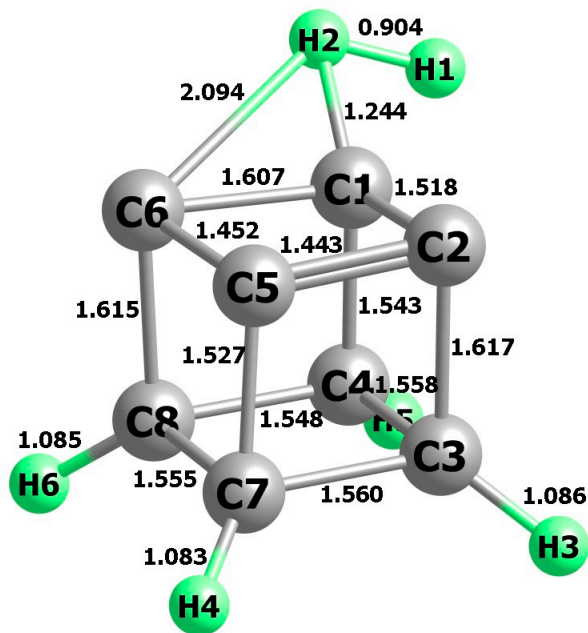


C_8H_2

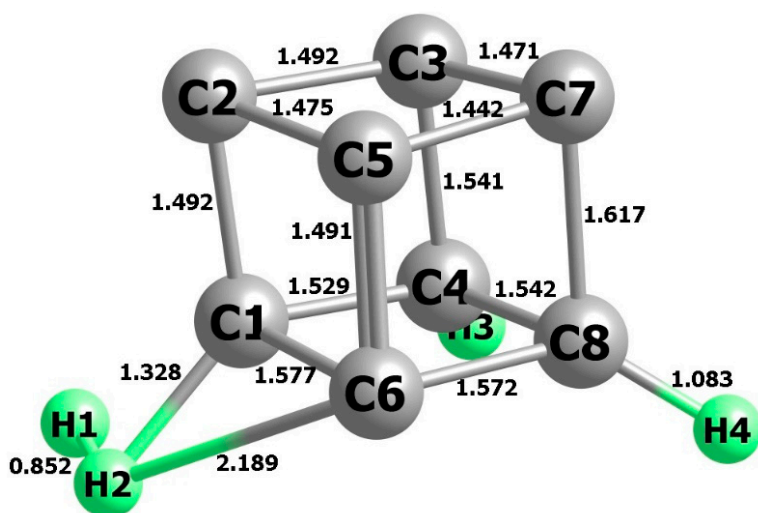
The images of transient states (TS1, TS2, TS3 and TS4)
of the cubane dehydrogenation reaction



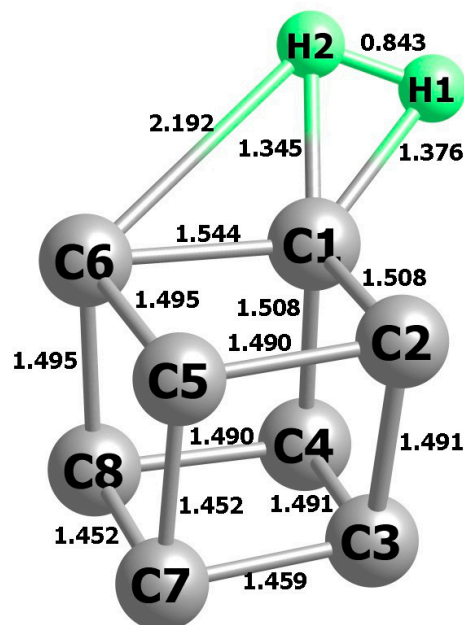
TS1



TS2



TS3



TS4