Theoretical Study on the Kinetics of the Reaction of C2H with C2H2

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**Table 1S**: Z-matrices and shapes of reactants, intermediates and transition states calculated by M06-2X/MG3S.

|  |  |  |
| --- | --- | --- |
|  | z-matrix | Shape |
| C2H | C  H,1,B1  C,1,B2,2,A1  Variables:  B1=1.06430511  B2=1.19621079  A1=180. |  |
| C2H2 | C  H,1,B1  C,1,B2,2,A1  H,2,B3,1,A2,3,D1,0  Variables:  B1=1.06320598  B2=1.19341078  B3=3.31982267  A1=180.  A2=0.00000148  D1=0. |  |
| INT3 | C  C,1,B1  C,2,B2,1,A1  C,3,B3,2,A2,1,D1,0  H,3,B4,2,A3,1,D2,0  H,4,B5,3,A4,2,D3,0  H,1,B6,2,A5,3,D4,0  Variables:  B1=1.1984596  B2=1.43181097  B3=1.31195555  B4=1.08645506  B5=1.0779091  B6=1.06303623  A1=179.40770065  A2=123.04657927  A3=116.82709616  A4=135.93490896  A5=179.86050348  D1=179.99870718  D2=0.00928328  D3=0.005335  D4=-179.83223842 |  |
| INT4 | C  C,1,B1  C,2,B2,1,A1  C,3,B3,2,A2,1,D1,0  H,3,B4,2,A3,1,D2,0  H,4,B5,3,A4,2,D3,0  H,1,B6,2,A5,3,D4,0  Variables:  B1=1.29245295  B2=1.44485012  B3=1.30375324  B4=1.07623266  B5=1.07588393  B6=1.07307754  A1=152.02809772  A2=63.6528077  A3=147.43884138  A4=149.15199093  A5=138.67472114  D1=179.99550607  D2=0.01415719  D3=-179.97692158  D4=-179.99269365 |  |
| INT5 | C  C,1,B1  C,2,B2,1,A1  C,3,B3,2,A2,1,D1,0  H,3,B4,2,A3,1,D2,0  H,4,B5,3,A4,2,D3,0  H,1,B6,2,A5,3,D4,0  Variables:  B1=1.43156121  B2=1.43107703  B3=1.41634651  B4=1.07465249  B5=1.08805474  B6=1.07467872  A1=93.95250213  A2=78.3202081  A3=136.39240781  A4=127.41132045  A5=136.34653137  D1=-27.85009698  D2=-178.36397811  D3=-118.75435601  D4=178.23712359 |  |
| P2 | C  C,1,B1  C,2,B2,1,A1  C,3,B3,2,A2,1,D1,0  H,3,B4,2,A3,1,D2,0  H,4,B5,3,A4,2,D3,0  H,2,B6,1,A5,3,D4,0  Variables:  B1=1.29360258  B2=1.46747242  B3=1.30818603  B4=1.08445146  B5=1.0776606  B6=1.10148855  A1=135.40395003  A2=123.90170795  A3=115.87636315  A4=136.99811338  A5=103.65177095  D1=-179.98522654  D2=0.00587647  D3=-0.00404965  D4=-179.98030753 |  |
| INT7 | C  C,1,B1  C,2,B2,1,A1  C,3,B3,2,A2,1,D1,0  H,4,B4,3,A3,2,D2,0  H,1,B5,2,A4,3,D3,0  H,4,B6,3,A5,2,D4,0  Variables:  B1=1.22206881  B2=1.32499861  B3=1.29917462  B4=1.08687463  B5=1.06262456  B6=1.08687517  A1=179.99448755  A2=179.99562206  A3=121.66600906  A4=179.95434946  A5=121.66617162  D1=0.  D2=-178.23735043  D3=0.  D4=1.71899277 |  |
| P8 | C  C,1,B1  C,2,B2,1,A1  C,3,B3,2,A2,1,D1,0  H,4,B4,3,A3,2,D2,0  H,1,B5,2,A4,3,D3,0  Variables:  B1=1.19905389  B2=1.37568417  B3=1.19905422  B4=1.06306428  B5=1.06306456  A1=179.99999915  A2=180.  A3=180.  A4=179.99999829  D1=0.  D2=0.  D3=0. |  |
| TS3/4 | C  C,1,B1  C,2,B2,1,A1  C,3,B3,2,A2,1,D1,0  H,3,B4,2,A3,1,D2,0  H,4,B5,3,A4,2,D3,0  H,1,B6,2,A5,3,D4,0  Variables:  B1=1.23477616  B2=1.42429728  B3=1.29685791  B4=1.08156619  B5=1.07858047  B6=1.06289498  A1=170.18227355  A2=80.72140408  A3=135.87299472  A4=148.17220113  A5=165.62787104  D1=179.22029894  D2=-0.78786698  D3=179.77219252  D4=-178.79806517 |  |
| TS4/5 | C  C,1,B1  C,2,B2,1,A1  C,1,B3,2,A2,3,D1,0  H,3,B4,2,A3,1,D2,0  H,4,B5,1,A4,2,D3,0  H,1,B6,4,A5,3,D4,0  Variables:  B1=1.2382278  B2=1.39002009  B3=2.10681422  B4=1.06978317  B5=1.09287418  B6=1.0636354  A1=140.14312579  A2=55.28803496  A3=136.08824728  A4=95.37106702  A5=131.00968576  D1=-1.54305231  D2=-156.39271086  D3=-121.71741717  D4=-175.18361853 |  |
| TS3/2 | C  C,1,B1  C,2,B2,1,A1  C,3,B3,2,A2,1,D1,0  H,3,B4,2,A3,1,D2,0  H,4,B5,3,A4,2,D3,0  H,2,B6,1,A5,3,D4,0  Variables:  B1=1.25074405  B2=1.43630862  B3=1.30920591  B4=1.08763849  B5=1.07699699  B6=1.3766201  A1=176.49600994  A2=125.60683676  A3=113.90236115  A4=137.3643259  A5=54.33159566  D1=179.88210803  D2=-0.11527714  D3=-0.0019462  D4=179.76293488 |  |
| TS3/7 | C  C,1,B1  C,2,B2,1,A1  C,3,B3,2,A2,1,D1,0  H,3,B4,2,A3,1,D2,0  H,4,B5,3,A4,2,D3,0  H,1,B6,2,A5,3,D4,0  Variables:  B1=1.20459576  B2=1.37962673  B3=1.28738615  B4=1.25997553  B5=1.08761747  B6=1.06288322  A1=174.73707998  A2=159.62470181  A3=138.57976504  A4=143.71320751  A5=179.29156483  D1=-179.93620148  D2=0.08021353  D3=0.17025848  D4=-179.48632491 |  |
| TS3/8 | C  C,1,B1  C,2,B2,1,A1  C,3,B3,2,A2,1,D1,0  H,3,B4,2,A3,1,D2,0  H,4,B5,3,A4,2,D3,0  H,1,B6,2,A5,3,D4,0  Variables:  B1=1.19812464  B2=1.38635854  B3=1.21431915  B4=1.79329604  B5=1.06377538  B6=1.06310799  A1=179.73130062  A2=161.02604096  A3=93.19936523  A4=171.42478077  A5=179.75027195  D1=-176.81087509  D2=3.15550223  D3=-179.85795557  D4=179.04678541 |  |
| TS7/8 | C  C,1,B1  C,2,B2,1,A1  C,3,B3,2,A2,1,D1,0  H,4,B4,3,A3,2,D2,0  H,1,B5,2,A4,3,D3,0  H,4,B6,3,A5,2,D4,0  Variables:  B1=1.20054187  B2=1.37022529  B3=1.20740649  B4=1.064084  B5=1.06325913  B6=1.99309231  A1=179.90948544  A2=176.57237082  A3=168.31382999  A4=179.9463519  A5=106.00129052  D1=150.98576778  D2=179.76113776  D3=125.24654727  D4=-0.54529369 |  |

**Table 2S.** Vibrational wave numbers and moments of inertia Ii for the intermediates and transition states of the reaction HC2 + C2H2 calculated with M06-2X/MG3S method.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| INT3 | INT4 | INT5 | INT7 | TS3/4 | TS3/7 | TS3/8 | TS4/5 | TS7/8 |
| Vibrational | frequencies | cm-1 |  |  |  |  |  |  |
| |  | | --- | | 3383.6 | | 3109.4 | | 2948.0 | | 2178.1 | | 1592.4 | | 1240.1 | | 961.2 | | 862.4 | | 818.5 | | 690.0 | | 721.1 | | 718.9 | | 508.2 | | 359.7 | | 214.6 | | Moments | | |  | | --- | | 3194.4 | | 3145.0 | | 3102.7 | | 1808.4 | | 1612.1 | | 1024.6 | | 991.0 | | 870.2 | | 846.2 | | 766.1 | | 666.3 | | 651.0 | | 488.8 | | 389.1 | | 361.8 |   of inertia | |  | | --- | | 3134.0 | | 3130.7 | | 2919.5 | | 1271.5 | | 1282.7 | | 1215.2 | | 1063.4 | | 1004.4 | | 993.3 | | 900.7 | | 790.8 | | 700.9 | | 604.3 | | 537.3 | | 528.7 |   amu Å2 | |  | | --- | | 3310.9 | | 2972.3 | | 2927.5 | | 1968.6 | | 1762.2 | | 1386.6 | | 957.8 | | 898.3 | | 872.0 | | 633.7 | | 550.2 | | 394.4 | | 617.0 | | 243.8 | | 200.1 | | 744.1**i**   |  | | --- | | 3309.5 | | 3085.3 | | 3015.5 | | 1904.6 | | 1636.2 | | 1141.5 | | 942.1 | | 849.2 | | 725.8 | | 583.7 | | 475.9 | | 482.6 | | 380.6 | | 341.4 | | |  | | --- | | 2173.3**i** | | 3369.0 | | 2878.0 | | 2271.6 | | 2126.4 | | 1815.3 | | 892.6 | | 823.1 | | 697.1 | | 585.8 | | 525.9 | | 380.9 | | 337.8 | | 223.1 | | 284.4 | | |  | | --- | | 1038.5**i** | | 3378.0 | | 3356.9 | | 2228.9 | | 2026. | | 908.2 | | 609.2 | | 703.1 | | 553.3 | | 447.7 | | 267.8 | | 635.8 | | 733.9 | | 551.6 | | 266.7 | | |  | | --- | | 111.7**i** | | 3159.5 | | 3139.8 | | 2846.2 | | 1795.8 | | 1313.7 | | 1107.1 | | 988.7 | | 893.3 | | 820.5 | | 851.7 | | 765.0 | | 404.3 | | 389.7 | | 328.1 | | |  | | --- | | 862.4i | | 3375.9 | | 3373.3 | | 2244.1 | | 2078.3 | | 907.3 | | 631.5 | | 713.4 | | 775.9 | | 737.9 | | 533.3 | | 547.9 | | 285.4 | | 243.3 | | 178.1 | |
| |  | | --- | | 9.862 | | 99.043 | | 108.906 | | |  | | --- | | 15.694 | | 66.621 | | 82.315 | | |  | | --- | | 25.519 | | 37.536 | | 58.760 | | |  | | --- | | 1.724 | | 121.185 | | 122.909 | | |  | | --- | | 15.064 | | 73.364 | | 88.428 | | |  | | --- | | 2.525 | | 117.633 | | 120.158 | | |  | | --- | | 4.683 | | 113.858 | | 118.541 | | |  | | --- | | 20.442 | | 52.315 | | 70.162 | | |  | | --- | | 4.614 | | 120.204 | | 124.818 | |

**Table 3S.** Overall reaction rate constants (cm-3 molecule-1 s-1) at different temperatures in comparison with some available experimental data.

|  |  |  |  |
| --- | --- | --- | --- |
| ***T (K)*** | ***k*** | ***Experimental*** | ***Reference*** |
| 143 | 1.260 × 10-10 | 1.79 × 10-10 | 22 |
| 160 | 1.269 × 10-10 | 1.54 × 10-10 | 22 |
| 170 | 1.277 × 10-10 | 1.3 × 10-10 | 20 |
| 180 | 1.287 × 10-10 | 1.28 × 10-10 | 20 |
| 200 | 1.309 × 10-10 | 1.26 × 10-10 | 20 |
| 220 | 1.335 × 10-10 | 1.25 × 10-10 | 20 |
| 240 | 1.362 × 10-10 | 1.24 × 10-10 | 20 |
| 260 | 1.391 × 10-10 | 1.22 × 10-10 | 20 |
| 280 | 1.420 × 10-10 | 1.22 × 10-10 | 20 |
| 298 | 1. 447 × 10-10 | 1.51 × 10-10  1.35 × 10-10  1.50 × 10-10  1.60 × 10-10 | 16  15  17  19 |
| 500 | 1.746 × 10-10 | 1.89 × 10-10  1.60 × 10-10 | 15  19 |
| 700 | 2.020 × 10-10 | 2.16 × 10-10  1.60 × 10-10 | 15  19 |
| 1000 | 2.389 × 10-10 | 2.39 × 10-10  1.50 × 10-10 | 15  17 |
| 1200 | 2.613 × 10-10 | 2.48 × 10-10  1.50 × 10-10 | 15  17 |
| 1400 | 2.823 × 10-10 | 2.55 × 10-10 | 15 |

Steady-state approximation to the activated intermediates:

(1)

(2)

(3)

(4)

from (1):

from (4):

from (3) :

(2):

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from (4) : [

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