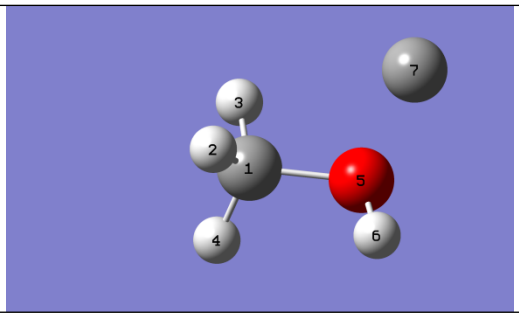
Electronic Supplementary Material (ESI) for RSC Advances.


**Supporting information file for "The fast C($^3$P) + $CH_3OH$ reaction as an efficient loss process for gas-phase interstellar methanol."**

**Quantum Chemical Calculations**

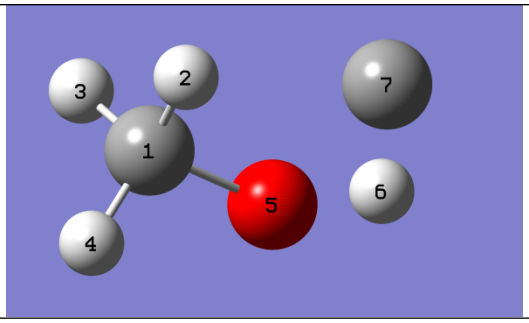
C + $CH_3OH$ theoretical calculations, geometries and frequencies (distances in Angstrom, angles in degrees, Frequencies in $cm^{-1}$ without corrections factors)

| | |
|---|---|
| complex1 |  |



| | M06-2X/cc-pVQZ | CCSD(T)-F12/aug-cc-pVTZ |
|---|---|---|
| $H_2$-$C_1$ | 1.0872 | 1.0885 |
| $H_3$-$C_1$ | 1.0838 | 1.0849 |
| $H_4$-$C_1$ | 1.0870 | 1.0887 |
| $O_5$-$C_1$ | 1.4362 | 1.4440 |
| $H_6$-$O_5$ | 0.9636 | 0.9645 |
| $C_7$-$O_5$ | 1.6895 | 1.7444 |
| $H_3$-$C_1$-$H_2$ | 106.70 | 109.91 |
| $H_4$-$C_1$-$H_3$ | 110.70 | 110.62 |
| $O_5$-$C_1$-$H_4$ | 109.18 | 108.89 |
| $H_6$-$O_5$-$C_1$ | 110.81 | 109.61 |
| $C_7$-$O_5$-$H_6$ | 104.29 | 101.92 |
| Diedre($H_4$-$C_1$-$H_3$-$H_2$) | 123.62 | 123.59 |
| Diedre($O_5$-$C_1$-$H_4$-$H_3$) | -115.85 | -115.68 |
| Diedre($H_6$-$O_5$-$C_1$-$H_4$) | -63.05 | -63.84 |
| Diedre($C_7$-$O_5$-$H_6$-$C_1$) | 119.22 | 116.71 |

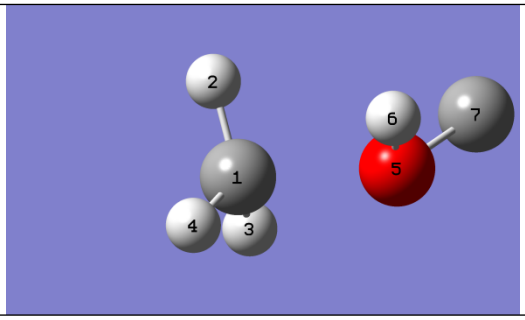
**Frequencies ($cm^{-1}$):**
M06-2X/cc-pVQZ:
151, 301, 441, 652, 1041, 1073, 1182, 1342, 1468, 1490, 1509, 3072, 3158, 3185, 3836
CCSD(T)/aug-cc-pVTZ:
158, 259, 368, 633, 1004, 1067, 1176, 1350, 1469, 1500, 1512, 3054, 3142, 3177, 3782

| TS1 |  |
|---|---|



| | M06-2X/cc-pVQZ | CCSD(T)-F12/aug-cc-pVTZ |
|---|---|---|
| $H_2$-$C_1$ | 1.0884 | 1.0894 |
| $H_3$-$C_1$ | 1.0864 | 1.0873 |
| $H_4$-$C_1$ | 1.0857 | 1.0873 |
| $O_5$-$C_1$ | 1.4353 | 1.4457 |
| $H_6$-$O_5$ | 1.1673 | 1.1727 |
| $C_7$-$O_5$ | 1.5588 | 1.6000 |
| $H_3$-$C_1$-$H_2$ | 109.62 | 108.89 |
| $H_4$-$C_1$-$H_3$ | 110.81 | 110.92 |
| $O_5$-$C_1$-$H_4$ | 107.91 | 107.58 |
| $H_6$-$O_5$-$C_1$ | 112.85 | 111.22 |
| $C_7$-$O_5$-$C_1$ | 113.00 | 111.55 |
| Diedre($H_4$-$C_1$-$H_3$-$H_2$) | 122.93 | 123.31 |
| Diedre($O_5$-$C_1$-$H_4$-$H_3$) | -117.42 | -117.11 |
| Diedre($H_6$-$O_5$-$C_1$-$H_4$) | -102.96 | -101.44 |
| Diedre($C_7$-$O_5$-$C_1$-$H_6$) | -61.50 | -58.75 |

**Frequencies ($cm^{-1}$):**
M06-2X/cc-pVQZ:
1495i, 191, 358, 700, 849, 1027, 1188, 1210, 1469, 1494, 1509, 2244, 3072, 3159, 3172
CCSD(T)-F12/aug-cc-pVTZ:
1544i, 115, 333, 625, 841, 982, 1169, 1196, 1456, 1494, 1503, 2213, 3047, 3141, 3155

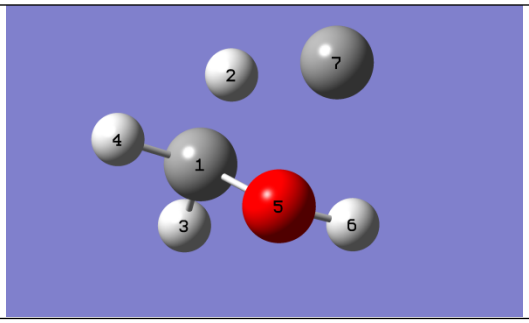
| TS3 |  |
|---|---|



| | M06-2X/cc-pVQZ | CCSD(T)-F12/aug-cc-pVTZ |
|---|---|---|
| $H_2$-$C_1$ | 1.0802 | 1.0827 |
| $H_3$-$C_1$ | 1.0787 | 1.0806 |

| | | |
|---|---|---|
| $H_4$-$C_1$ | 1.0811 | 1.0833 |
| $O_5$-$C_1$ | 1.7940 | 1.8078 |
| $H_6$-$O_5$ | 0.9723 | 0.9735 |
| $C_7$-$O_5$ | 1.3878 | 1.4035 |
| $H_3$-$C_1$-$H_2$ | 115.30 | 115.46 |
| $H_4$-$C_1$-$H_3$ | 115.77 | 115.95 |
| $O_5$-$C_1$-$H_4$ | 105.31 | 104.88 |
| $H_6$-$O_5$-$C_1$ | 101.65 | 100.07 |
| $C_7$-$O_5$-$C_1$ | 116.70 | 117.35 |
| Diedre($H_4$-$C_1$-$H_3$-$H_2$) | 140.95 | 141.66 |
| Diedre($O_5$-$C_1$-$H_4$-$H_3$) | -106.45 | -106.34 |
| Diedre($H_6$-$O_5$-$C_1$-$H_4$) | -63.47 | -61.95 |
| Diedre($C_7$-$O_5$-$C_1$-$H_6$) | -119.18 | -116.49 |

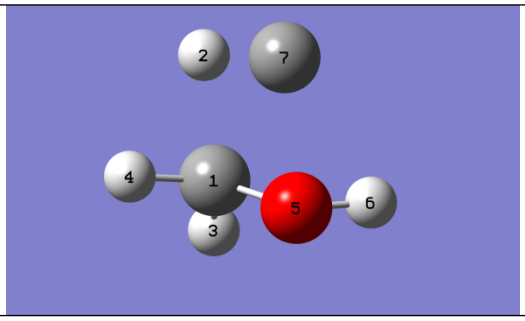
**Frequencies ($cm^{-1}$):**
M06-2X/cc-pVQZ:
1050i, 162, 296, 705, 771, 875, 928, 1112, 1174, 1437, 1457, 3101, 3259, 3272, 3626
CCSDT/aug-cc-pVTZ:
1199i, 131, 287, 694, 725, 838, 903, 1097, 1156, 1443, 1454, 3081, 3236, 3253, 3604

| | |
|---|---|
| Complex2 |  |



| | M06-2X/cc-pVQZ | CCSD(T)-F12/aug-cc-pVTZ |
|---|---|---|
| $H_2$-$C_1$ | 1.1661 | 1.1545 |
| $H_3$-$C_1$ | 1.0876 | 1.0894 |
| $H_4$-$C_1$ | 1.0892 | 1.0896 |
| $O_5$-$C_1$ | 1.3761 | 1.3888 |
| $H_6$-$O_5$ | 0.9626 | 0.9622 |
| $C_7$-$O_5$ | 2.8177 | 2.9223 |
| $H_3$-$C_1$-$H_2$ | 108.01 | 108.06 |
| $H_4$-$C_1$-$H_3$ | 111.16 | 111.14 |
| $O_5$-$C_1$-$H_4$ | 109.07 | 108.64 |
| $H_6$-$O_5$-$C_1$ | 108.60 | 108.00 |
| $C_7$-$O_5$-$C_1$ | 53.21 | 53.05 |
| Diedre($H_4$-$C_1$-$H_3$-$H_2$) | 109.03 | 111.17 |
| Diedre($O_5$-$C_1$-$H_4$-$H_3$) | -128.13 | -126.90 |
| Diedre($H_6$-$O_5$-$C_1$-$H_4$) | -175.85 | -177.48 |
| Diedre($C_7$-$O_5$-$C_1$-$H_6$) | 33.64 | 34.80 |

**Frequencies ($cm^{-1}$):**
M06-2X/cc-pVQZ:
183, 241, 365, 577, 1028, 1112, 1162, 1346, 1386, 1484, 1584, 2231, 3089, 3157, 3847
CCSD(T)-F12/aug-cc-pVDZ:
126, 181, 310, 479, 1016, 1105, 1130, 1346, 1290, 1471, 1519, 2287, 3063, 3136, 3803

| TS4 |  |
|---|---|



| | M06-2X/cc-pVQZ | CCSD(T)-F12/aug-cc-pVTZ |
|---|---|---|
| $H_2$-$C_1$ | 1.4395 | 1.4682 |
| $H_3$-$C_1$ | 1.0887 | 1.0903 |
| $H_4$-$C_1$ | 1.0890 | 1.0899 |
| $O_5$-$C_1$ | 1.3561 | 1.3623 |
| $H_6$-$O_5$ | 0.9650 | 0.9661 |
| $C_7$-$O_5$ | 2.5613 | 2.5699 |
| $H_3$-$C_1$-$H_2$ | 113.25 | 112.63 |
| $H_4$-$C_1$-$H_3$ | 111.92 | 112.70 |
| $O_5$-$C_1$-$H_4$ | 109.46 | 109.48 |
| $H_6$-$O_5$-$C_1$ | 108.42 | 107.55 |
| $C_7$-$O_5$-$C_1$ | 45.81 | 45.93 |
| Diedre($H_4$-$C_1$-$H_3$-$H_2$) | 97.19 | 97.18 |
| Diedre($O_5$-$C_1$-$H_4$-$H_3$) | -131.91 | -132.48 |
| Diedre($H_6$-$O_5$-$C_1$-$H_4$) | -173.38 | -174.20 |
| Diedre($C_7$-$O_5$-$C_1$-$H_6$) | 37.40 | 38.92 |

**Frequencies ($cm^{-1}$):**
M06-2X/cc-pVQZ:
610i, 254, 432, 566, 619, 855, 1136, 1207, 1237, 1387, 1491, 2387, 3091, 3165, 3803
CCSDT/aug-cc-VTZ:
613i, 226, 393, 515, 569, 835, 1117, 1166, 1205, 1390, 1487, 2468, 3055, 3140, 3745

**Table S1** Reaction enthalpies in kJ $mol^{-1}$ (at 0 K including ZPE) of species involved in the C + methanol reaction by different methods.

| | Complex1 | TS1 | TS3 | Complex2 | TS4 |
|---|---|---|---|---|---|
| MRCI+Q/avtz// CASSCF/avtz | -27 | +23 | +42 | +21 | +43 |
| CCSDT-F12/avtz | -51 | +3 | +18 | -9 | -3 |
| M06/vqz | -69 | -17 | -1 | -26 | -20 |
| CASPT2/avqz// CASSCF/avqz | -50 | -28 | -15 | -29 | -38 |

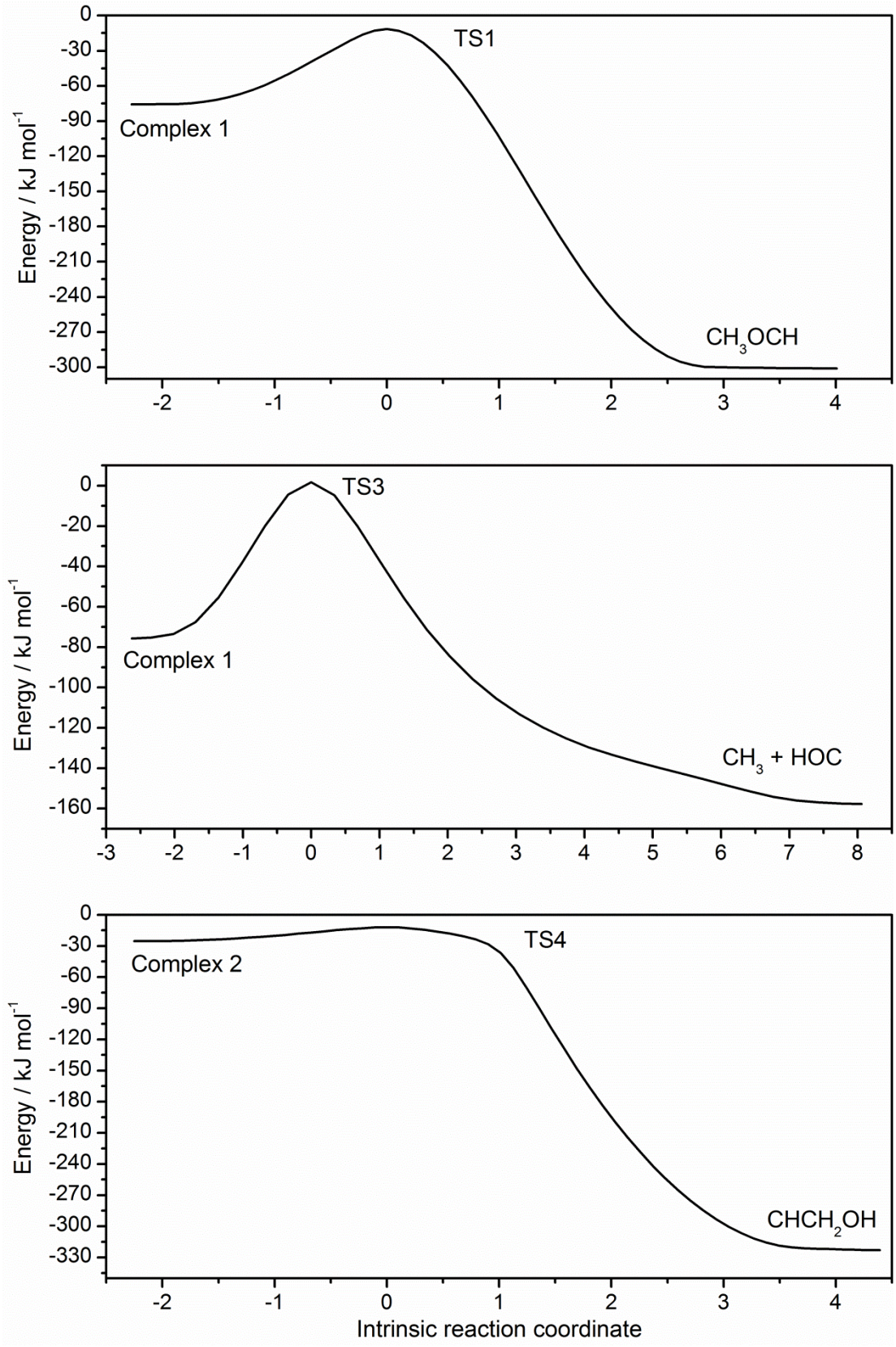



**Figure S1** Potentials along the minimum energy path leading from complex1 and complex2 to adducts/products.