Table S-1: Calculated Vibrational Frequencies of the Transition State at the B3LYP/6-31G(d,p) Level of Theory[a]

TS(I)

-480, 3, 30, 37, 64, 71, 98, 139, 156, 189, 207, 238, 276, 325, 375, 403, 423, 462, 485, 494, 507, 572, 579, 582, 623, 695, 699, 710, 731, 732, 754, 784, 815, 826, 914, 934, 951, 1001, 1069, 1073, 1088, 1180, 1242, 1265, 1367, 1381, 1386, 1461, 1467, 1509, 1566, 1652, 1679, 1867, 1919, 2394, 3588, 3646, 3677,

TS(II)

-346, 61, 126, 205, 254, 366, 404, 431, 473, 550, 587, 614, 701, 751, 809, 836, 887, 984, 998, 1075, 1195, 1207, 1337, 1392, 1470, 1667, 1693, 1896, 3430, 3668,

TS(III)

-437, 63, 101, 121, 181, 268, 297, 382, 454, 490, 543, 584, 688, 719, 763, 798, 841, 885, 976, 1139, 1215, 1358, 1388, 1405, 1512, 1639, 1688, 1950, 3368, 3542,

TS(IV)

-1155, 113, 183, 255, 320, 439, 539, 569, 698, 763, 846, 900, 1108, 1138, 1296, 1470, 1696, 1842, 1933, 3492,

TS(V)

-525, 105, 297, 432, 447, 564, 646, 749, 847, 900, 1339, 1576, 1905, 3534, 3668,

[a] All frequencies are in $cm^{-1}$, and the negative numbers indicate imaginary frequencies

# Table S-2

**Total Energies(hartrees) and Zero-Point Energies(kcal $mol^{-1}$) for Reactant, Products, and Transition State (6-31G Level)**

| Molecule | Total Energies | ZEP |
|---|---|---|
| NTO isolated molecule | -518.85093 | 45.88419 |
| NTO 2 molecule (Optimized) | -1037.71682 | 92.57786 |
| NO($CN_3H_2CO$) (nitoroso-TO) | -444.08140 | 42.50166 |
| $NO_2$($CN_3OH_2CO$)(a new triazole) | -593.57948 | 48.05280 |
| [2NTO → NO($CN_3H_2CO$) + $NO_2$($CN_3OH_2CO$)] ‡ | -1037.62722 | 90.35878 |