Supplementary Information

Computational Study on Reaction Mechanisms and Kinetics of RNCN (R =H, F, Cl, Br, CH_3) Radicals with NO

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Table S1. Frequencies and moments of inertia for the species involved in the reaction of RNCN (R =H, F, Cl, Br, CH_3) + NO, calculated at the B3LYP/6-311++G(3df,2p) level

Species	Vibrational wavenumbers (cm^{-1})	Moments of inertia (amu $bohr^2$)
HNCN	309.8, 446.0, 449.7, 1250.5 , 1765.0 , 3388.2	2.76, 160.91 , 163.67
NO	1979.3	0.00, 34.93, 34.93
HIM1	78.5, 173.1, 360.6, 464.1, 576.3, 678.3, 812.1, 845.3, 1280.4, 1682.8, 2159.4, 3611.3	105.64, 487.75, 574.17
HIM6	281.3, 428.3, 646.7, 767.8, 770.3, 857.7, 929.3, 1081.6, 1188.7, 1540.2, 1853.3, 3532.7	112.70, 303.02, 415.73
FNCN	244.0, 410.6, 657.2, 947.4, 1071.5, 2070.4	33.39, 338.12, 371.50
FIM1	51.0, 117.0, 198.7, 263.5, 292.6, 561.4, 655.8, 731.2, 873.7, 1286.8, 1876.0, 2083.5	101.08, 1179.35, 1218.74
FIM6	191.22, 217.4, 420.3, 491.1, 671.6, 748.0, 834.6, 1009.5, 1092.8, 1214.6, 1505.7, 1770.1	112.01, 1676.51, 1728.97
ClNCN	210.4, 435.8, 565.8, 716.3, 1109.0, 2030.7	42.88, 530.52, 573.39
ClIM1	63.1, 101.9, 182.1, 218.3, 299.2, 571.4, 605.2, 682.7, 737.7, 1318.0, 1804.0, 2104.2	112.01, 1676.51, 1728.97
ClIM6	168.5, 175.4, 390.3, 422.3, 627.7, 710.3, 751.8, 883.9, 1082.1, 1146.5, 1513.3, 1777.1	143.38, 988.15, 1131.53
BrNCN	184.4, 444.5, 476.9, 669.5, 1124.4, 1999.0	50.63, 771.19, 821.82
BrIM1	59.9, 94.5, 170.4, 197.7, 308.8, 490.6, 601.9, 659.9, 742.5, 1313.6, 1780.5, 2097.2	134.15, 2403.67, 2476.36
BrIM6	144.2, 156.1, 358.3, 374.1, 596.7, 665.6, 752.5, 853.1, 1076.3, 1115.1, 1520.0, 1779.7	149.23, 1535.7, 1684.94
CNNCN	157.1, 428.7, 444.8, 485.9, 628.5, 903.5, 1325.5, 1924.5, 2175.0	34.91, 614.92, 649.83
CNIM1	64.7, 88.1, 149.2, 169.9, 289.2, 490.1, 502.4, 578.9, 608.8, 700.0, 903.0, 1469.9, 1851.2, 2200.9, 2337.1	92.21, 1774.67, 1823.40
CNIM6	127.6, 137.7, 313.9, 417.4, 500.5, 568.0, 595.7, 760.4, 784.3, 1071.3, 1106.2, 1157.5, 1536.5, 1827.9, 2313.3	141.35, 1041.26, 1182.60
NH_2NCN	250.9, 378.3, 436.4, 546.4, 668.0, 966.7, 1259.1, 1372.8, 1652.2, 2164.9, 3500.4, 3669.7	143.11, 948.77, 1024.62
NH_2IM1	53.7, 134.7, 217.5, 259.9, 303.0, 359.3, 569.7, 647.7, 769.3, 807.6, 1016.5, 1285.7, 1415.3, 1670.0, 1700.8, 2155.4, 3474.1, 3595.0	118.36, 318.87, 437.22

NH_2IM6	183.3, 210.8, 403.9, 489.1, 512.6, 553.5, 672.9, 732.0, 795.7, 1071.9, 1183.9, 1235.8, 1324.7, 1452.6, 1667.1, 1781.0, 3508.7, 3667.5	133.94, 626.57, 759.44
CH_3NCN	47.2, 228.3, 453.3, 639.2, 887.8, 1073.0, 1147.4, 1260.0, 1431.5, 1467.7, 1493.5, 1927.8, 3011.2, 3066.6, 3098.7	36.49, 361.75, 387.21
CH_3IM1	46.3, 78.4, 108.6, 161.3, 222.0, 424.2, 617.2, 727.8, 786.5, 786.5, 920.8, 1133.3, 1150.0, 1360.5, 1456.9, 1489.8, 1501.5, 1612.7, 2253.5, 3038.5, 3110.6, 3113.4	153.29, 908.26, 1032.46
CH_3IM6	122.4, 186.0, 198.5, 393.2, 485.7, 620.9, 757.8, 765.2, 1041.2, 1058.9, 1111.1, 1129.8, 1179.0, 1437.3, 1487.9, 1499.5, 1527.0, 1861.8, 3028.8, 3099.0, 3103.3	141.03, 645.40, 775.36
HTS2	*i*576.2, 130.5, 134.9, 225.9, 354.6, 489.5, 624.6, 825.8, 1322.2, 1745.7, 2100.7, 3811.9	94.45, 529.08, 623.53
HTS3	*i*460.8, 228.0, 347.0, 541.0, 637.1, 711.3, 817.4, 1060.3, 1248.7, 1336.6, 2040.7, 3683.4	114.27, 351.67, 465.95
HTS9	*i*721.41, 181.4, 392.8, 627.6, 630.0, 711.5, 744.3, 911.9, 1114.4, 1799.5, 1857.0, 3621.3	127.93, 311.95, 439.88
FTS2	*i*285.1, 133.8, 144.4, 393.8, 461.3, 505.4, 633.9, 693.1, 778.5, 1353.4, 1650.9, 2168.0	113.24,332.64, 445.88
FTS3	*i*585.6, 142.7, 226.4, 325.1, 481.6, 673.1, 775.1, 1044.4, 1096.6, 1251.5, 1273.2, 1874.3	156.93, 708.33, 855.26
FTS9	*i*204.3, 93.0, 114.3, 258.2, 313.1, 510.7, 752.8, 969.9, 1322.5, 1555.6, 2428.2, 2721.5	144.15, 658.62, 802.77
ClTS2	*i*511.1, 42.1, 45.0, 161.6, 353.8, 439.3, 578.1, 665.9, 788.2, 1315.2, 1830.1, 2026.5	89.24, 1641.40, 1730.64
ClTS3	*i*472.9, 86.45, 115.8, 191.2, 352.7, 555.0, 672.7, 984.7, 1038.1, 1269.7, 1302.9, 2031.8	156.31, 1181.13, 1337.44
ClTS9	*i*616.7, 46.3, 172.3, 361.4, 388.8, 596.0, 660.0, 702.6, 780.6, 1098.0, 1674.3, 1863.7	143.78, 1042.35, 1186.13
BrTS2	*i*515.1, 34.8, 49.9, 141.6, 340.7, 420.6, 535.1, 577.8, 766.6, 1311.8, 1853.0, 2007.1	97.87, 2433.34, 2531.21
BrTS3	*i*472.4, 80.9, 94.3, 192.4, 349.6, 454.6, 678.6, 929.2, 1038.2, 1263.1, 1306.8, 2016.9	168.26, 1789.37, 1957.64
BrTS9	*i*615.3, 64.2, 135.9, 332.7, 337.8, 586.1, 644.5, 745.0, 1097.5, 1698.5, 1857.0	143.78, 1042.35, 1186.13
CNTS2	*i*571.2, 64.2, 67.4, 142.1, 225.2, 339.5, 470.3, 504.3, 608.5, 780.3, 1027.9, 1328.6, 1795.8, 2078.4, 2351.5	82.18, 1704.48, 1817.67

CNTS3	*i*456.7, 96.5, 132.7, 238.3, 352.3, 489.0, 497.7, 642.4, 694.0, 1064.1, 1150.5, 1253.9, 1310.1, 2075.8, 2350.0	146.99, 1209.51, 1356.50
CNTS9	*i*490.2, 87.4, 127.7, 288.8, 421.7, 486.8, 545.6, 691.5, 700.5, 785.9, 1004.8, 1224.4, 1757.7, 1849.4, 2318.7	136.74, 1104.64, 1241.38
NH_2TS2	*i*509.1, 60.4, 72.9, 135.1, 163.6, 332.6, 375.9, 609.0, 766.7, 811.3, 1100.4, 1313.4, 1334.7, 1660.6, 1752.3, 2223.8, 3480.8, 3574.6	101.38, 1096.60, 1195.62
NH_2TS3	*i*441.6, 121.6, 197.0, 199.4, 338.5, 369.3, 644.9, 700.0, 1031.1, 1195.8, 1258.9, 1320.7, 1356.0, 1664.0, 2123.2, 3484.4, 3603.5	147.42, 755.59, 900.36
NH_2TS9	*i*512.8, 116.5, 223.0, 432.9, 450.3, 503.3, 583.7, 638.0, 722.1, 902.6, 1106.6, 1219.9, 1308.2, 1563.1, 1649.0, 1817.2, 3482.8, 3658.6	143.12, 642.53, 782.66
CH_3TS2	*i*541.9, 21.8, 74.1, 86.3, 177.7, 291.9, 343.6, 622.5, 773.6, 992.2, 1143.9, 1148.7, 1313.0, 1455.4, 1486.4, 1489.4, 1743.0, 2241.3, 3044.6, 3114.8, 3121.6	107.48, 1113.75, 1209.88
CH_3TS3	*i*428.6, 105.1, 137.5, 183.7, 281.5, 420.7, 659.3, 712.1, 1068.9, 1079.7, 1143.4, 1149.1, 1204.7, 1375.6, 1453.6, 1487.5, 1495.5, 2111.7, 3042.2, 3116.7, 3120.3	151.43, 734.21, 874.45
CH_3TS9	*i*596.1, 30.6, 104.1, 186.5, 359.6, 397.8, 671.9, 686.4, 718.7, 971.3, 1119.8, 1142.3, 1161.6, 1440.5, 1489.9, 1503.1, 1786.2, 1902.3, 3032.6, 3094.6, 3114.1	142.87, 693.23, 824.84

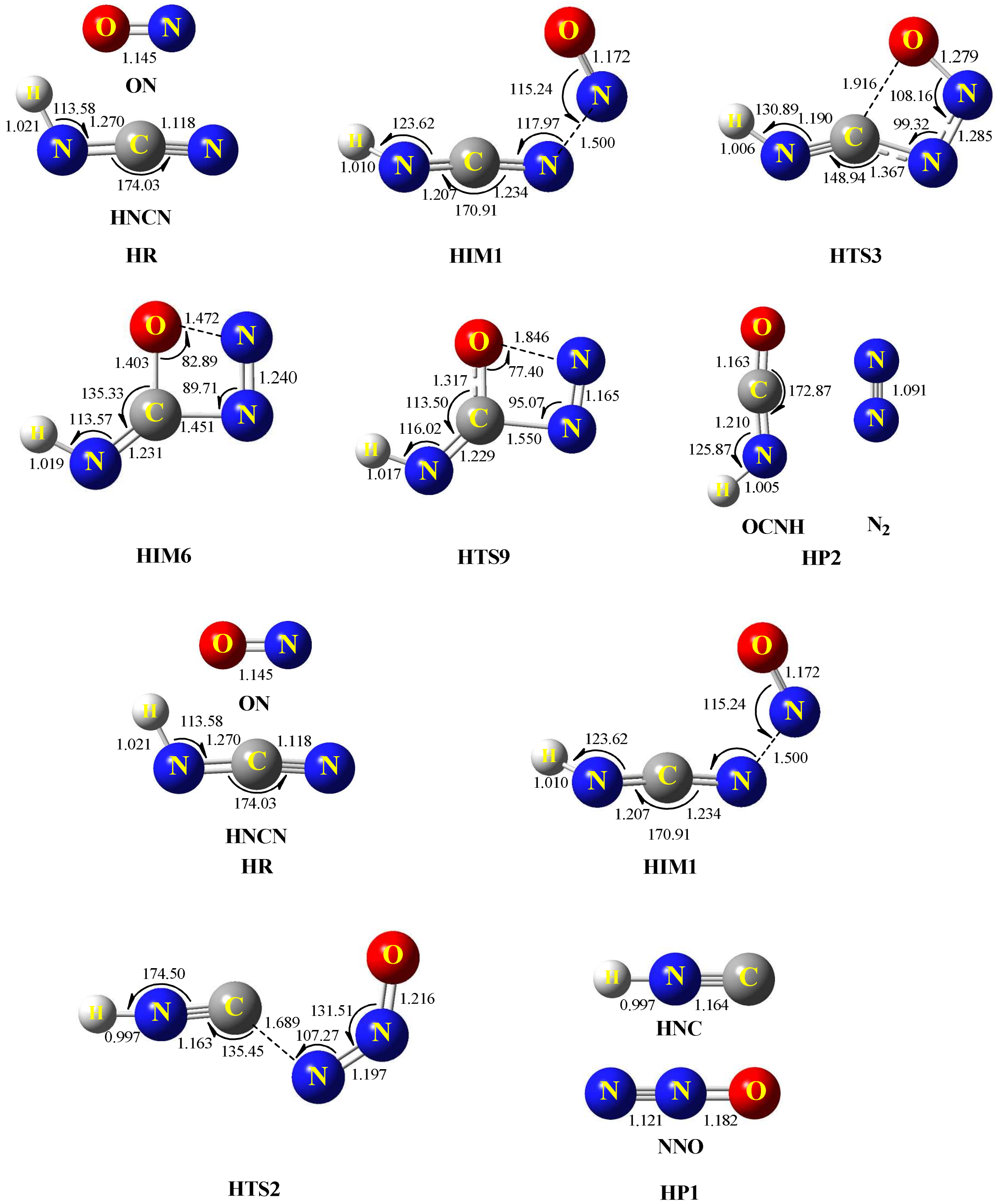


Figure S1. The calculated structural parameters of all involved stationary geometries of RNCN + NO (R = H) reaction at the B3LYP/6-311++G(3df,2p) level

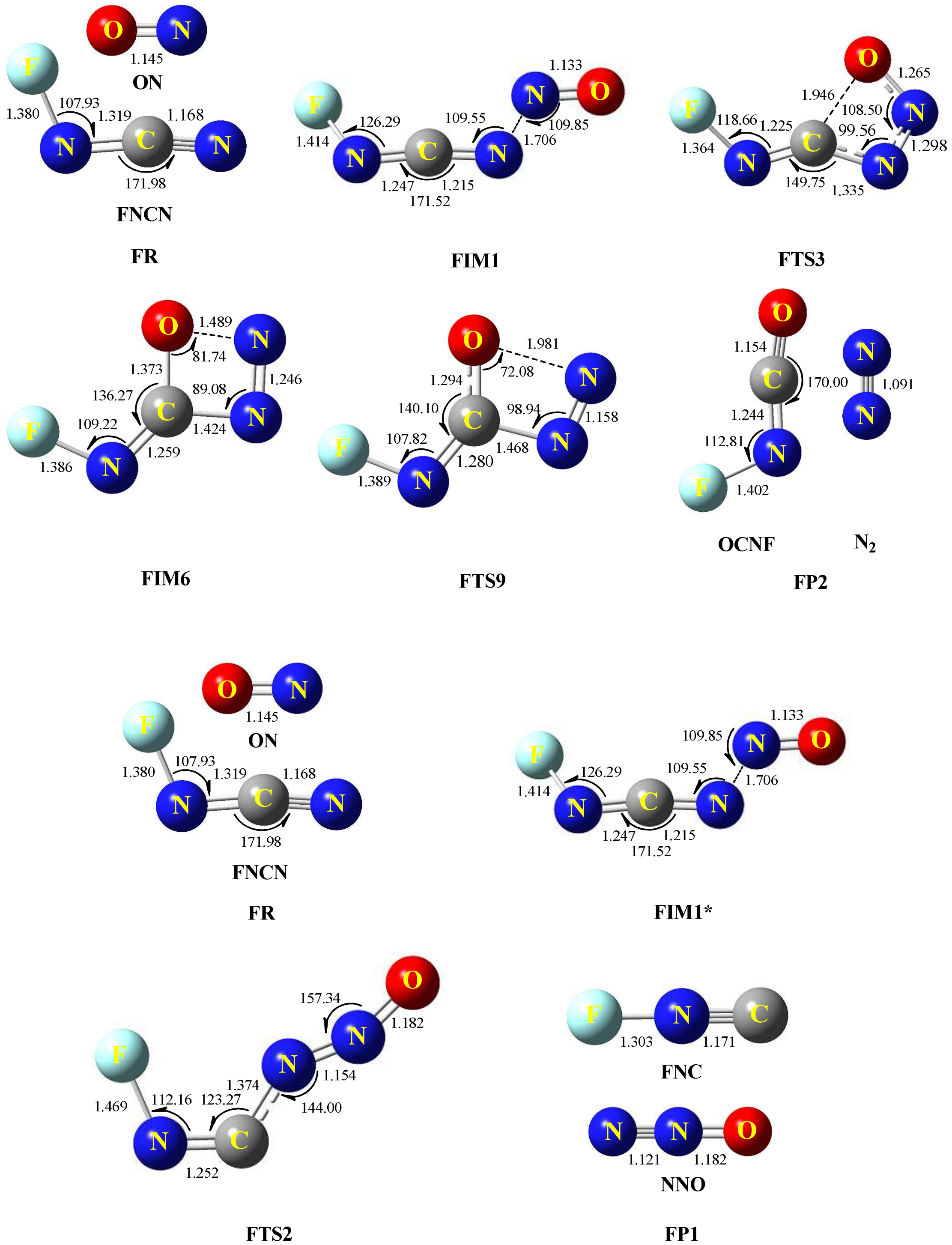
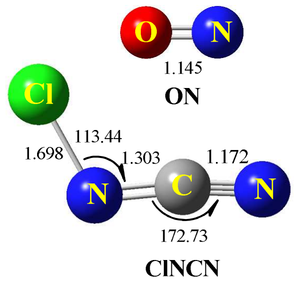
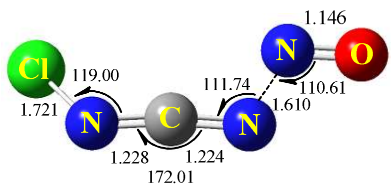


Figure S2. The calculated structural parameters of all involved stationary geometries of RNCN + NO (R = F) reaction at the B3LYP/6-311++G(3df,2p) level



ClR



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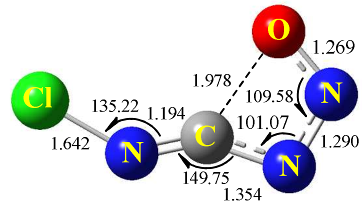

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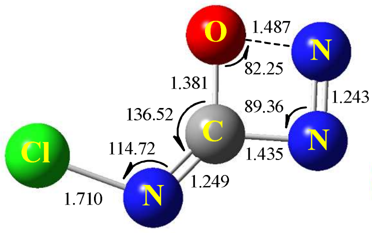

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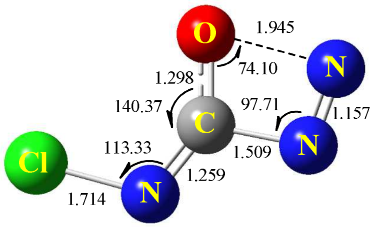

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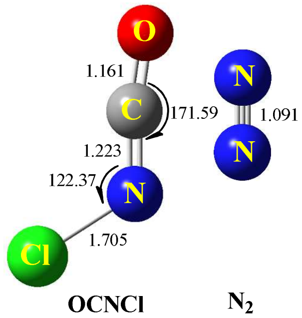

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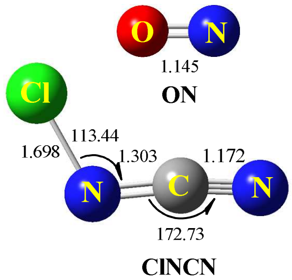

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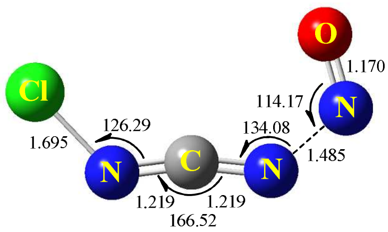

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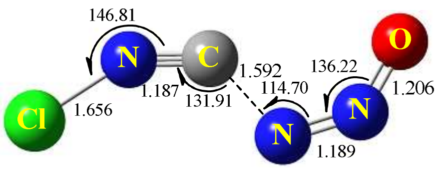

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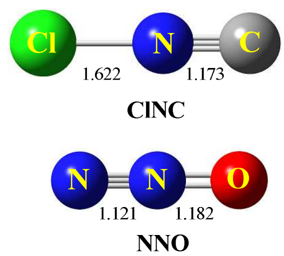

ClP1

Figure S3. The calculated structural parameters of all involved stationary geometries of RNCN + NO (R = Cl) reaction at the B3LYP/6-311++G(3df,2p) level

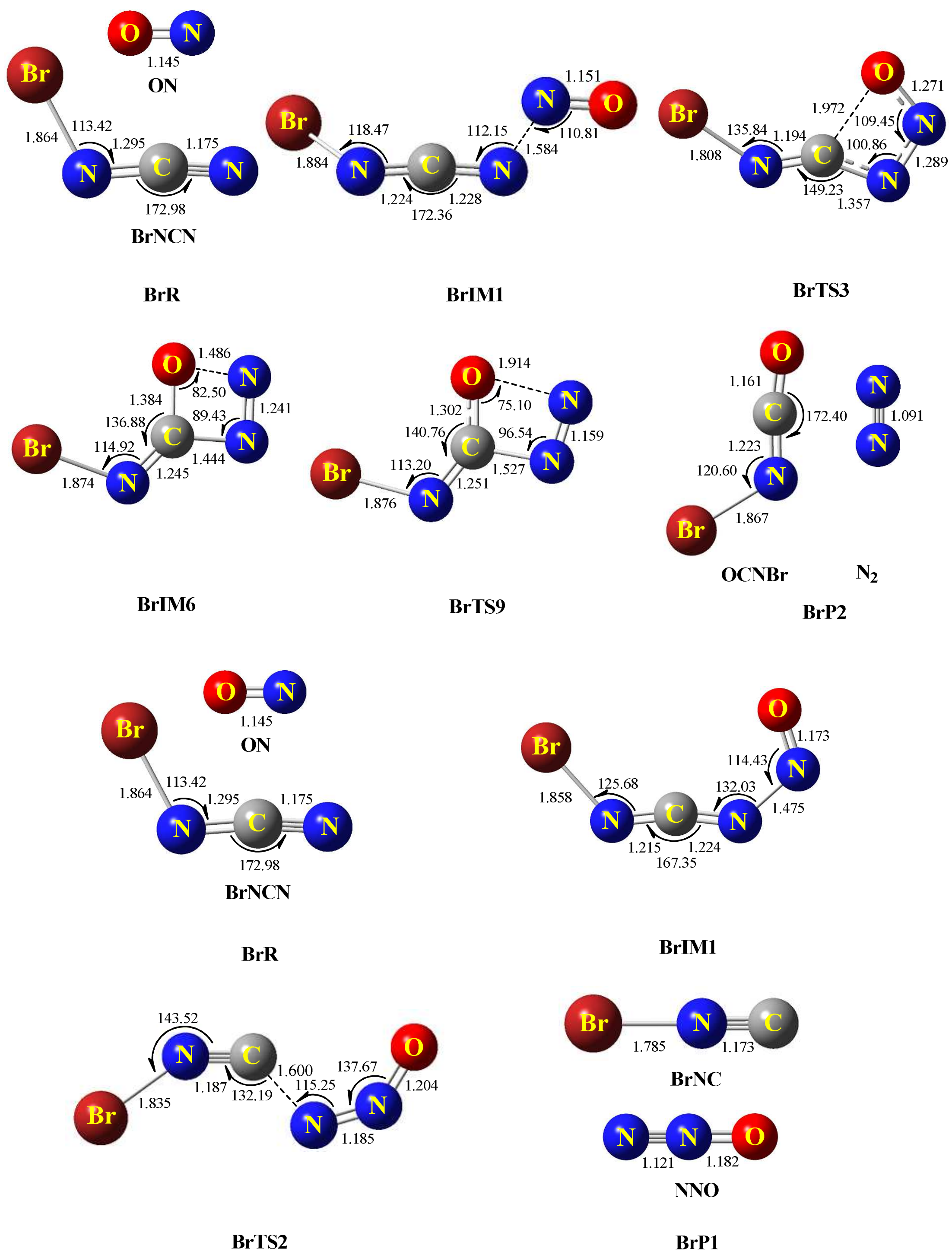

Figure S4. The calculated structural parameters of all involved stationary geometries of RNCN + NO (R = Br) reaction at the B3LYP/6-311++G(3df,2p) level

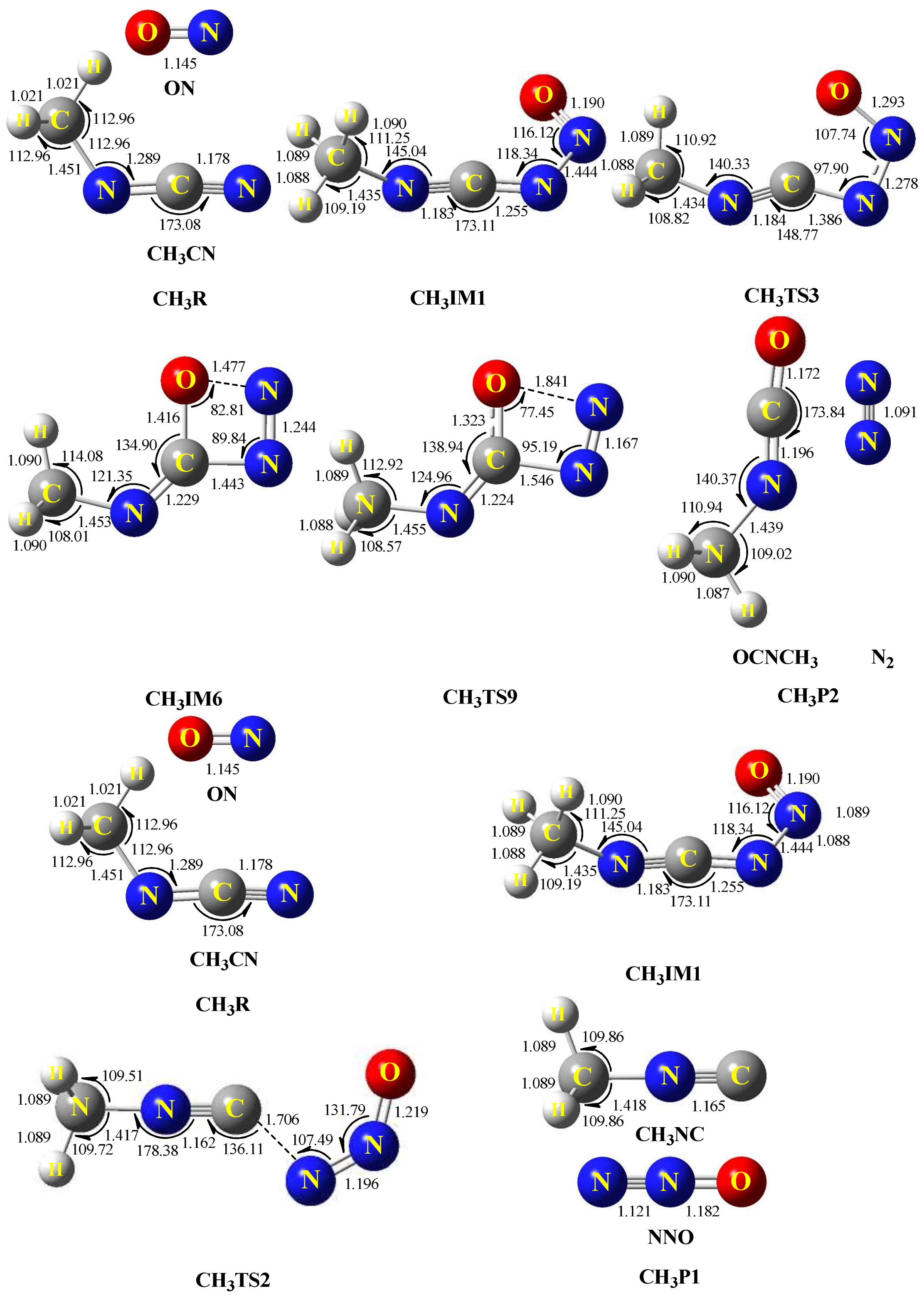

Figure S5. The calculated structural parameters of all involved stationary geometries of RNCN + NO (R = CH_3) reaction at the B3LYP/6-311++G(3df,2p) level