

Supporting information

Atmospheric Oxidation Mechanism and Kinetics of 2-Bromo-4, 6-dinitroaniline by OH radical – A Theoretical Study

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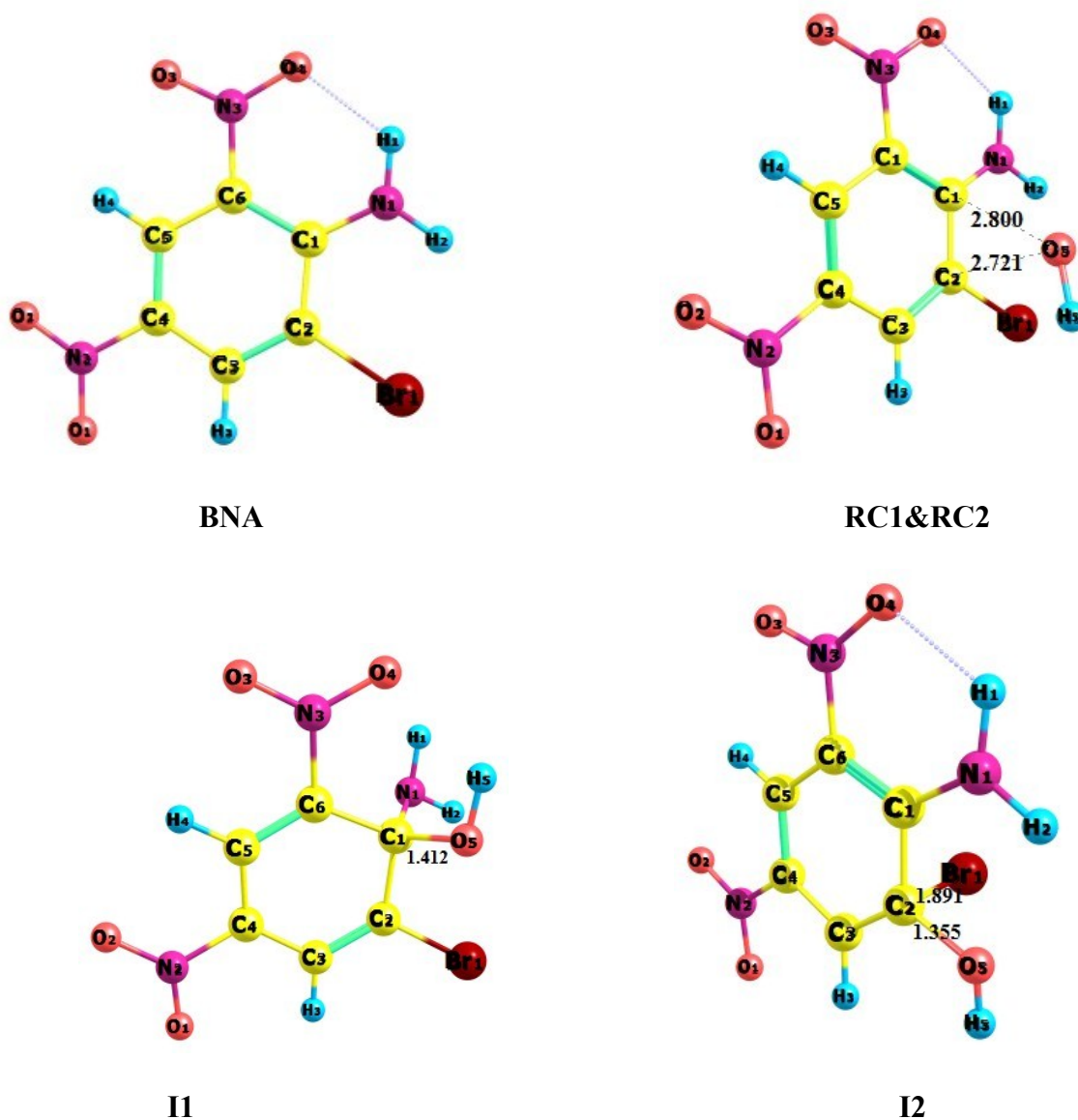
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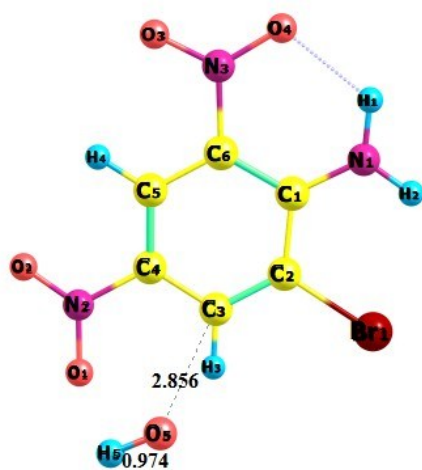
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Dublin 4, Ireland.

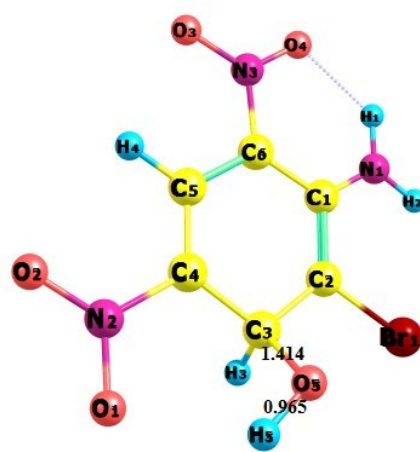
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Fig. S1: The optimized structure of the reactant, reactant complexes, intermediate complexes and intermediates involved in the initial reaction of BNA with OH radical.

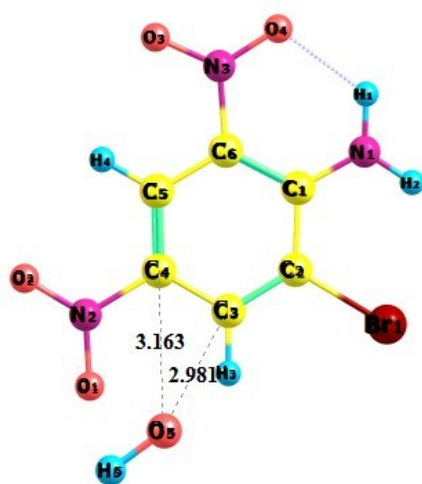




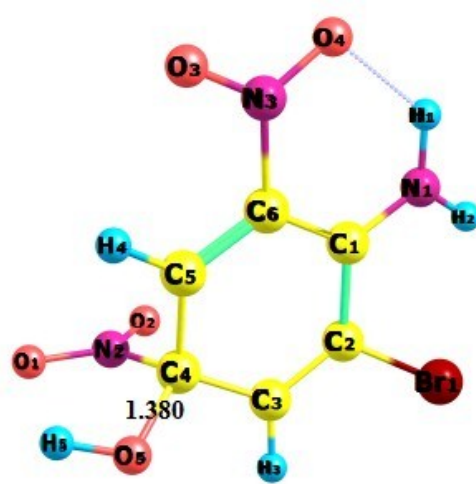
RC3



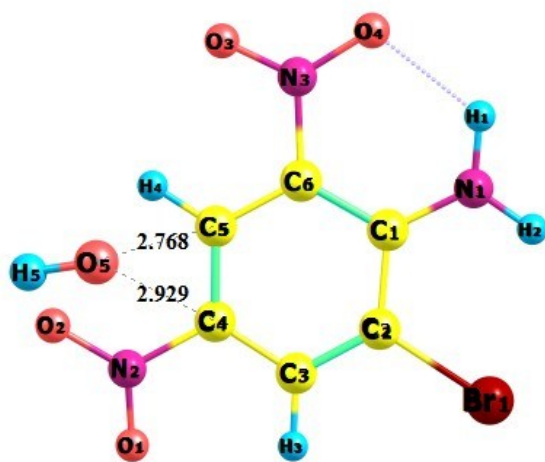
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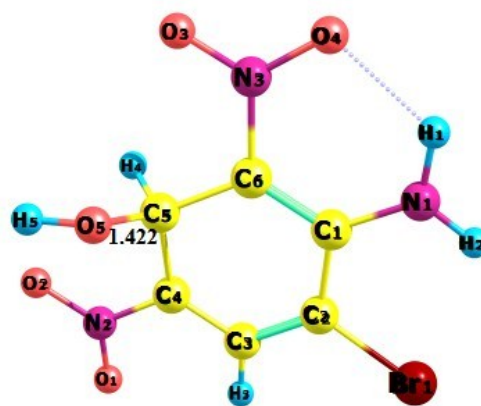
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I4



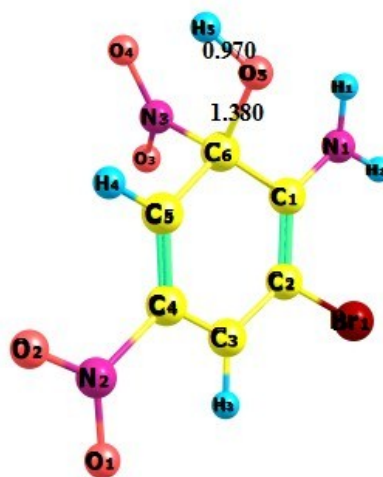
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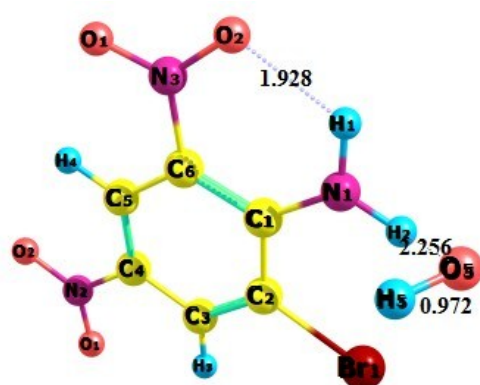
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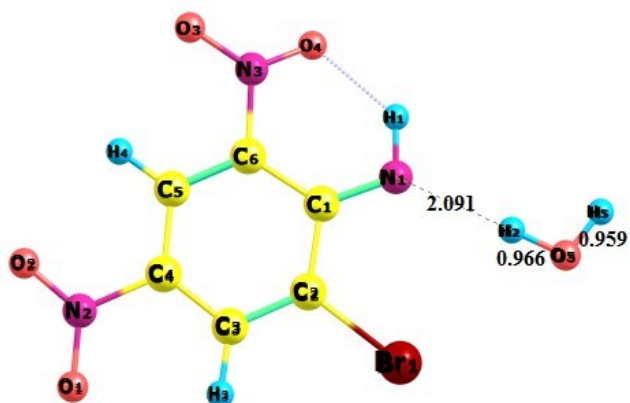
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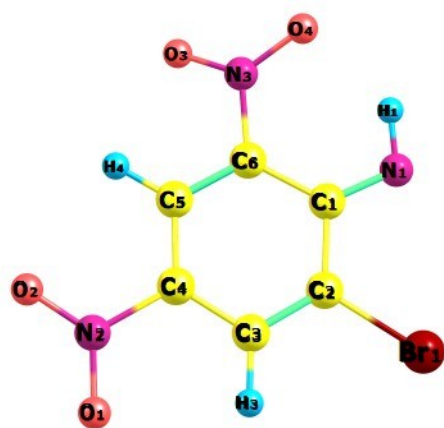
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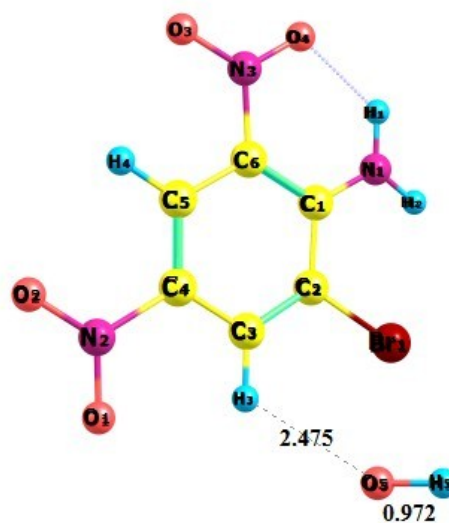
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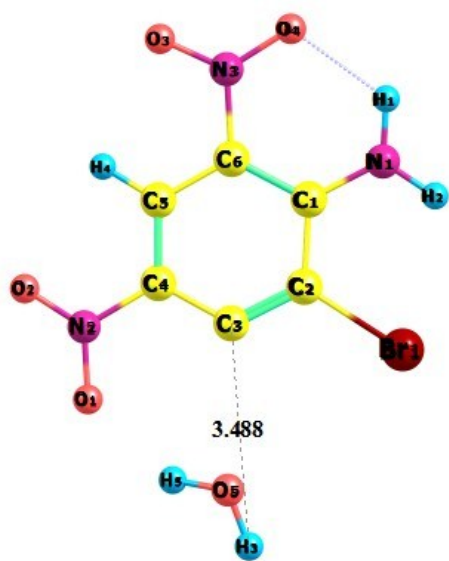
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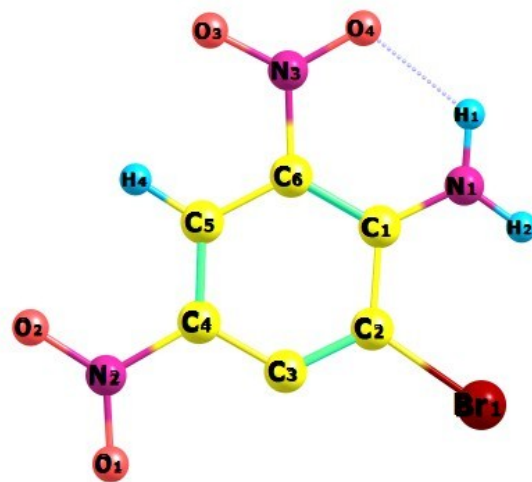
I7



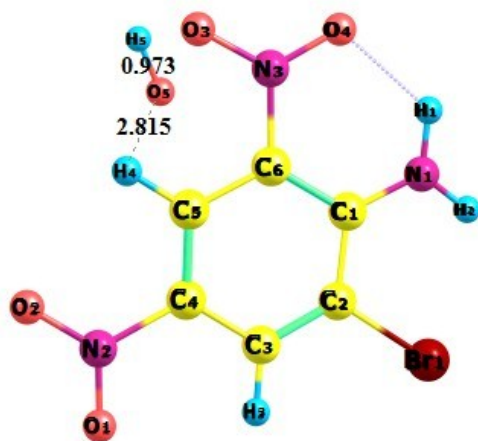
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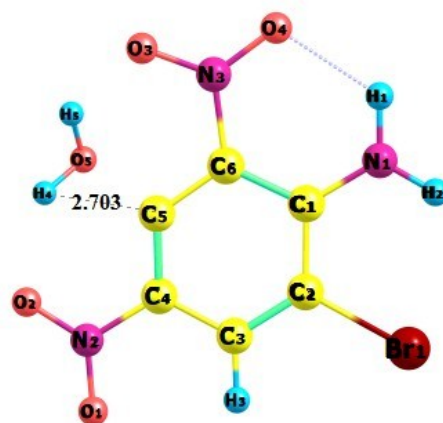
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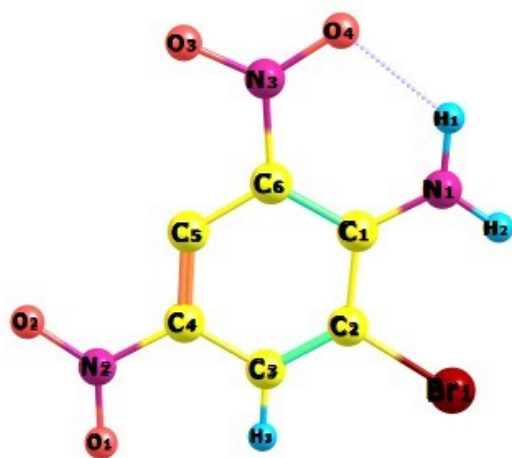
I8



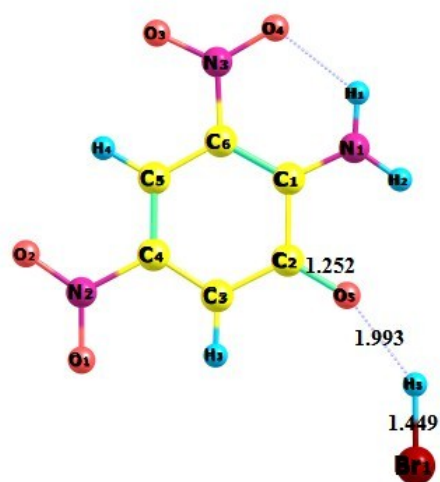
RC9



IC3



I9



I10

Table S1: Harmonic vibrational frequencies of isolated reactant, reactant complex, transition states, intermediate complexes and intermediate for the initial reactions calculated at M06-2X/6-311++G(d, p) level of theory.

Reactive species	Vibrational Frequencies (cm ⁻¹)
BNA	51, 52, 84, 120, 148, 180, 197, 281, 303, 319, 355, 361, 394, 436, 445, 481, 551, 621, 636, 648, 721, 729, 737, 756, 850, 901, 927, 962, 974, 1072, 1108, 1184, 1245, 1336, 1381, 1438, 1455, 1467, 1521, 1609, 1640, 1670, 1711, 1720, 3218, 3248, 3603, 3735
RC1	41, 51, 52, 56, 90, 116, 146, 148, 180, 195, 207, 281, 304, 329, 355, 362, 393, 419, 438, 447, 489, 552, 619, 637, 657, 724, 729, 745, 756, 850, 902, 923, 965, 974, 1076, 1107, 1183, 1246, 1342, 1379, 1439, 1453, 1467, 1521, 1610, 1639, 1672, 1711, 1717, 3215, 3248, 3602, 3731, 3769
TS1	-589i , 33, 45, 75, 79, 108, 150, 173, 197, 208, 240, 281, 310, 350, 376, 383, 427, 451, 481, 515, 550, 624, 634, 645, 723, 727, 752, 761, 800, 839, 898, 931, 962, 966, 1089, 1101, 1180, 1245, 1337, 1361, 1440, 1445, 1454, 1485, 1578, 1613, 1660, 1707, 1717, 3230, 3248, 3586, 3694, 3817
I1	38, 45, 94, 111, 145, 163, 190, 230, 256, 274, 305, 310, 353, 372, 409, 448, 461, 500, 545, 549, 643, 655, 715, 723, 734, 756, 800, 820, 884, 923, 953, 965, 1044, 1067, 1107, 1152, 1177, 1243, 1289, 1349, 1400, 1426, 1430, 1447, 1538, 1626, 1651, 1692, 1705, 3232, 3239, 3535, 3626, 3836
TS2	-510i , 51, 54, 84, 95, 136, 148, 170, 184, 208, 219, 279, 311, 353, 361, 395, 415, 437, 489, 519, 549, 639, 651, 693, 726, 730, 750, 753, 797, 849, 900, 914, 962, 971, 1067, 1109, 1181, 1246, 1354, 1366, 1440, 1444, 1455, 1514, 1593, 1619, 1670, 1706, 1719, 3222, 3247, 3573, 3704, 3809
I2	24, 43, 52, 58, 82, 121, 142, 174, 231, 279, 304, 341, 359, 374, 404, 429, 437, 462, 488, 499, 574, 647, 659, 667, 724, 739, 744, 839, 855, 905, 954, 968, 996, 1110, 1142, 1172, 1271, 1322, 1345, 1424, 1451, 1457, 1494, 1543, 1613, 1648, 1677, 1713, 1719, 3234, 3261, 3603, 3737, 3897
RC3	41, 51, 52, 56, 90, 116, 146, 148, 180, 195, 207, 281, 304, 329, 355, 362, 393, 419, 438, 447, 489, 552, 619, 637, 657, 724, 729, 745, 756, 850, 902, 923, 965, 974, 1076, 1107, 1183, 1246, 1342, 1379, 1439, 1453, 1467, 1521, 1610, 1639, 1672, 1711, 1717, 3215, 3248, 3602, 3731, 3769
TS3	-673i , 42, 56, 82, 90, 116, 127, 155, 182, 208, 284, 330, 352, 356, 363, 377, 401, 435, 477, 509, 576, 612, 644, 706, 728, 738, 750, 767, 829, 860, 900, 958, 967, 999, 1072, 1098, 1177, 1241, 1316, 1367, 1428, 1436, 1444, 1510, 1571, 1627, 1655, 1698, 1707, 3222, 3244, 3614, 3745, 3748
I3	45, 52, 82, 96, 123, 156, 183, 216, 249, 280, 330, 335, 343, 378, 389, 433, 470, 486, 512, 602, 621, 652, 672, 715, 727, 735, 747, 826, 891, 935, 977, 1047, 1071, 1112, 1156, 1220, 1237, 1288, 1333, 1357, 1381, 1424, 1435, 1446, 1525, 1645, 1657, 1673, 1717, 3003, 3236, 3592, 3735, 3860
RC4	30, 43, 53, 75, 83, 133, 149, 169, 182, 225, 282, 310, 326, 355, 358, 363, 364, 393, 436, 463, 528, 562, 625, 639, 694, 730, 743, 754, 767, 852, 902, 946, 974, 977, 1078, 1114, 1186, 1255, 1343, 1385, 1442, 1446, 1475, 1524, 1610, 1637, 1674, 1705, 1716, 3239, 3242, 3599, 3733, 3742
TS4	-509i , 40, 65, 84, 94, 102, 150, 166, 191, 235, 282, 298, 302, 358, 365, 395, 410, 437, 459, 487, 550, 638, 651, 697, 726, 740, 750, 771, 809, 846, 898, 925, 938, 959, 1074, 1098, 1172, 1252, 1341, 1380, 1436, 1461, 1485, 1516, 1587, 1623, 1674, 1713, 1725, 3234, 3248, 3588, 3719, 3783
I4	33, 49, 59, 75, 81, 177, 215, 244, 286, 293, 298, 325, 363, 376, 383, 420, 424, 438, 464, 552, 581, 592, 638, 665, 714, 739, 745, 811, 837, 849, 861, 888, 945, 1042, 1085, 1221, 1226, 1256, 1309, 1363, 1412, 1449, 1463, 1510, 1553, 1614, 1687, 1722, 1728, 3221, 3248, 3590, 3722, 3775

RC5	3, 39, 52, 63, 93, 120, 148, 152, 178, 207, 241, 283, 318, 335, 349, 363, 384, 418, 430, 470, 515, 552, 593, 639, 684, 727, 735, 757, 772, 852, 900, 939, 957, 975, 1080, 1107, 1186, 1245, 1344, 1386, 1446, 1452, 1472, 1525, 1613, 1639, 1676, 1710, 1716, 3228, 3238, 3607, 3737, 3750
TS5	-528i , 50, 59, 85, 87, 112, 141, 151, 184, 200, 281, 329, 349, 357, 366, 375, 392, 438, 473, 506, 566, 640, 642, 711, 722, 742, 757, 774, 797, 855, 900, 936, 964, 1005, 1071, 1098, 1179, 1244, 1340, 1368, 1430, 1441, 1445, 1517, 1574, 1599, 1659, 1691, 1698, 3226, 3244, 3588, 3727, 3770
I5	45, 69, 88, 118, 123, 155, 180, 195, 234, 276, 280, 337, 344, 378, 392, 398, 439, 482, 512, 598, 638, 657, 679, 712, 738, 752, 777, 824, 890, 933, 943, 1025, 1077, 1111, 1166, 1236, 1250, 1284, 1337, 1360, 1386, 1418, 1442, 1445, 1549, 1575, 1656, 1668, 1687, 3088, 3214, 3581, 3736, 3869
RC6	9, 39, 52, 63, 93, 121, 148, 152, 178, 207, 242, 283, 318, 335, 349, 363, 384, 417, 430, 471, 515, 552, 592, 639, 684, 727, 735, 757, 772, 852, 900, 939, 957, 975, 1080, 1107, 1186, 1245, 1346, 1386, 1446, 1452, 1472, 1525, 1613, 1639, 1676, 1710, 1716, 3228, 3238, 3607, 3737, 3750
TS6	-438i , 52, 63, 81, 101, 143, 146, 169, 183, 209, 263, 282, 321, 353, 359, 386, 429, 437, 467, 538, 548, 628, 639, 723, 732, 738, 753, 789, 803, 847, 895, 941, 945, 967, 1074, 1096, 1173, 1243, 1353, 1392, 1441, 1449, 1455, 1518, 1600, 1634, 1674, 1714, 1726, 3232, 3241, 3578, 3710, 3801
I6	41, 57, 60, 80, 118, 149, 178, 226, 259, 297, 328, 341, 350, 364, 375, 399, 433, 495, 512, 521, 548, 595, 622, 693, 717, 742, 751, 809, 829, 849, 856, 879, 972, 1090, 1107, 1184, 1239, 1278, 1338, 1376, 1399, 1447, 1463, 1517, 1561, 1621, 1662, 1718, 1733, 3229, 3251, 3601, 3727, 3777
RC7	26, 36, 45, 48, 71, 110, 136, 143, 151, 182, 204, 281, 300, 316, 357, 366, 395, 440, 449, 482, 530, 553, 638, 657, 658, 721, 733, 739, 760, 851, 904, 939, 962, 974, 1081, 1112, 1185, 1251, 1334, 1382, 1439, 1452, 1468, 1523, 1612, 1637, 1672, 1711, 1717, 3236, 3248, 3582, 3706, 3791
TS7	-1668i , 41, 46, 48, 83, 110, 131, 149, 177, 197, 229, 278, 309, 344, 364, 372, 405, 466, 488, 523, 550, 641, 690, 716, 725, 749, 761, 768, 819, 851, 908, 940, 954, 971, 1110, 1127, 1186, 1250, 1321, 1354, 1434, 1452, 1454, 1477, 1505, 1628, 1645, 1710, 1725, 1770, 3237, 3239, 3555, 3828
IC1	23, 43, 47, 65, 70, 116, 127, 150, 169, 173, 183, 284, 305, 350, 359, 371, 394, 424, 456, 482, 494, 549, 645, 680, 712, 732, 747, 761, 808, 845, 899, 933, 950, 959, 1091, 1125, 1167, 1267, 1338, 1359, 1398, 1446, 1451, 1465, 1567, 1618, 1630, 1705, 1722, 3225, 3237, 3502, 3805, 3975
I7	52, 53, 66, 119, 151, 170, 186, 282, 305, 343, 359, 369, 421, 473, 491, 547, 641, 686, 713, 730, 742, 754, 789, 845, 896, 926, 957, 960, 1087, 1117, 1162, 1260, 1312, 1361, 1395, 1444, 1452, 1463, 1568, 1618, 1704, 1717, 3221, 3233, 3541
RC8	27, 42, 53, 70, 83, 120, 131, 142, 154, 182, 209, 281, 312, 332, 356, 361, 391, 396, 436, 455, 511, 552, 619, 637, 671, 725, 730, 742, 756, 850, 902, 949, 966, 974, 1075, 1111, 1185, 1251, 1336, 1381, 1438, 1456, 1469, 1521, 1611, 1637, 1673, 1712, 1719, 3243, 3246, 3609, 3739, 3788
TS8	-1653i , 38, 46, 52, 80, 113, 122, 177, 187, 197, 279, 289, 319, 324, 346, 353, 370, 425, 432, 461, 493, 587, 618, 631, 644, 652, 719, 731, 743, 765, 785, 877, 902, 942, 994, 1080, 1131, 1207, 1328, 1351, 1397, 1439, 1451, 1468, 1515, 1605, 1621, 1666, 1708, 1715, 3224, 3602, 3733, 3768
IC2	11, 45, 59, 81, 86, 113, 121, 166, 176, 181, 210, 277, 301, 310, 339, 355, 358, 391, 433, 454, 474, 513, 550, 629, 641, 650, 724, 729, 741, 753, 839, 899, 955, 966, 1079, 1118, 1207, 1326, 1353, 1433, 1447, 1454, 1515, 1596, 1607, 1621, 1665, 1700, 1709, 3243, 3591, 3723, 3845, 3979
I8	53, 64, 85, 117, 130, 172, 205, 275, 298, 329, 332, 353, 397, 435, 448, 491, 549, 617, 635, 642, 719, 725, 740, 751, 837, 898, 949, 966, 1075, 1114, 1206, 1323, 1353, 1433, 1449, 1453, 1515, 1607, 1625, 1668, 1707, 1714, 3232, 3602, 3733

RC9	25, 48, 61, 82, 86, 130, 147, 151, 182, 210, 231, 284, 319, 323, 338, 359, 363, 397, 439, 462, 520, 554, 619, 640, 688, 732, 735, 759, 764, 851, 904, 933, 954, 976, 1076, 1115, 1183, 1251, 1337, 1385, 1440, 1454, 1477, 1518, 1611, 1641, 1673, 1708, 1719, 3218, 3252, 3606, 3736, 3775
TS9	-1750i , 27, 47, 58, 82, 121, 156, 175, 201, 222, 277, 306, 322, 330, 343, 356, 383, 411, 433, 468, 515, 586, 600, 642, 677, 718, 730, 742, 765, 785, 826, 902, 926, 964, 1028, 1092, 1159, 1197, 1319, 1345, 1388, 1429, 1453, 1466, 1512, 1599, 1627, 1669, 1699, 1722, 3208, 3615, 3744, 3800
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H ₂ O	1595, 3894, 4000
OH	3766

Table S2: Cartesian coordinates of the transition states involved in the studied reactions calculated at M06-2X/6-311++G(d, p) level of theory.

Species	Reaction coordinates
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TS1	6	1.042590000	-0.954975000	-0.029366000
	6	-0.398089000	-1.021487000	-0.103177000
	6	1.712148000	0.279965000	-0.105011000
	1	2.791489000	0.299230000	-0.166150000
	6	-1.079548000	0.229111000	-0.053574000
	6	0.980777000	1.433028000	-0.051314000
	6	-0.420908000	1.427641000	-0.025757000
	1	-0.959886000	2.364948000	0.004086000
	7	1.876497000	-2.135213000	-0.376891000
	8	1.313190000	-3.188309000	-0.599544000
	8	3.070282000	-1.977323000	-0.407798000
	7	-1.067874000	-2.167521000	-0.129374000
	1	-0.562706000	-3.040969000	-0.159568000
	1	-2.074634000	-2.155501000	-0.075708000
	35	-2.971989000	0.227331000	-0.043430000
	7	1.681232000	2.725341000	-0.066863000
	8	0.996438000	3.725560000	-0.072280000
	8	2.891710000	2.704749000	-0.068683000
	8	1.055701000	-1.492045000	1.885427000
	1	1.755984000	-0.923300000	2.241519000
TS2	6	-0.997914000	1.099592000	-0.182521000
	6	0.448770000	1.002630000	-0.148013000
	6	-1.824998000	0.002342000	-0.121866000
	1	-2.898734000	0.127819000	-0.104021000
	6	0.950223000	-0.362561000	-0.110152000
	6	-1.254491000	-1.258403000	-0.078277000
	6	0.127183000	-1.455236000	-0.053620000
	1	0.526538000	-2.459356000	-0.008028000
	7	-1.656718000	2.414587000	-0.160651000
	8	-0.966254000	3.405658000	-0.301443000
	8	-2.855130000	2.433911000	-0.008754000
	7	1.263640000	1.987436000	-0.585013000
	1	0.906964000	2.927479000	-0.489255000
	1	2.243629000	1.863052000	-0.376527000
	35	2.808164000	-0.625004000	-0.092788000
	7	-2.135740000	-2.433997000	-0.030656000
	8	-1.604244000	-3.520817000	0.043988000
	8	-3.329492000	-2.236104000	-0.072135000
	8	0.494477000	1.279962000	1.784847000
	1	0.030081000	0.568895000	2.254323000
TS3	6	-1.066467000	1.159476000	-0.079511000
	6	0.351553000	1.105733000	-0.050429000
	6	-1.855801000	0.021823000	-0.074121000
	1	-2.933618000	0.111529000	-0.091000000
	6	0.925480000	-0.224506000	0.056938000
	6	-1.250005000	-1.220377000	-0.058250000
	6	0.126037000	-1.363852000	-0.051810000
	1	0.572291000	-2.348838000	-0.090438000
	7	-1.775084000	2.439888000	-0.116692000
	8	-1.109127000	3.464395000	-0.131999000

TS4	8	-2.981819000	2.420698000	-0.130598000
	7	1.159140000	2.157571000	-0.063262000
	1	0.765779000	3.087068000	-0.040997000
	1	2.152158000	2.013055000	0.042091000
	35	2.773276000	-0.437750000	-0.331635000
	7	-2.089548000	-2.425579000	-0.087263000
	8	-1.521300000	-3.496066000	-0.050066000
	8	-3.288551000	-2.269392000	-0.142658000
	8	1.024208000	0.037964000	2.058564000
	1	0.945089000	-0.875297000	2.375244000
	6	-1.041034000	1.251770000	-0.031240000
	6	0.380303000	1.227658000	-0.035991000
	6	-1.817120000	0.096886000	-0.127547000
	1	-2.895969000	0.172755000	-0.122428000
	6	0.961404000	-0.063852000	-0.172232000
	6	-1.198540000	-1.115537000	-0.222319000
	6	0.211868000	-1.242316000	-0.170924000
	1	0.675963000	-2.168553000	-0.481526000
	7	-1.782323000	2.507886000	0.086629000
	8	-1.146341000	3.548196000	0.168228000
TS5	8	-2.989439000	2.455668000	0.094420000
	7	1.161500000	2.314734000	0.042923000
	1	0.742212000	3.225107000	0.143047000
	1	2.161372000	2.201353000	0.072273000
	35	2.830178000	-0.232654000	-0.208046000
	7	-2.002841000	-2.331988000	-0.260628000
	8	-1.421517000	-3.380062000	-0.035153000
	8	-3.182538000	-2.229473000	-0.502635000
	8	0.447991000	-1.772731000	1.713475000
	1	-0.020724000	-2.622643000	1.642584000
	6	-0.778975000	1.210584000	-0.201346000
	6	0.617869000	1.083048000	-0.079665000
	6	-1.650103000	0.105243000	-0.173827000
	1	-2.687624000	0.259369000	-0.432926000
	6	1.112360000	-0.269963000	-0.060892000
	6	-1.081673000	-1.170070000	-0.218762000
	6	0.291612000	-1.365670000	-0.139765000
	1	0.692722000	-2.370283000	-0.136195000
	7	-1.427474000	2.510694000	-0.246947000
	8	-0.727922000	3.510600000	-0.150915000
	8	-2.627861000	2.542376000	-0.386723000
	7	1.477446000	2.106983000	-0.016187000
	1	1.120151000	3.050184000	-0.000802000
	1	2.463945000	1.924587000	0.067905000
	35	2.974127000	-0.554616000	0.070176000
	7	-1.964097000	-2.333457000	-0.265499000
	8	-1.457021000	-3.413229000	-0.472299000
	8	-3.151526000	-2.138484000	-0.088649000
	8	-2.094148000	-0.049786000	1.762118000

TS6	1	-2.883503000	-0.612681000	1.683566000
	6	1.042582000	-0.954936000	-0.029768000
	6	-0.398061000	-1.021481000	-0.103064000
	6	1.712083000	0.279932000	-0.105140000
	1	2.791427000	0.299344000	-0.166281000
	6	-1.079546000	0.229141000	-0.053655000
	6	0.980773000	1.433050000	-0.051388000
	6	-0.420907000	1.427672000	-0.025891000
	1	-0.959884000	2.364983000	0.003920000
	7	1.876540000	-2.135177000	-0.377042000
	8	1.313056000	-3.188300000	-0.599369000
	8	3.070190000	-1.977236000	-0.408217000
	7	-1.067832000	-2.167528000	-0.128608000
	1	-0.562651000	-3.040950000	-0.159289000
	1	-2.074612000	-2.155501000	-0.075404000
	35	-2.971991000	0.227365000	-0.043546000
	7	1.681266000	2.725322000	-0.066710000
	8	0.996486000	3.725554000	-0.071851000
	8	2.891746000	2.704666000	-0.068636000
	8	1.055678000	-1.492228000	1.885626000
	1	1.756782000	-0.923895000	2.240716000
	6	-0.761755000	1.320572000	-0.134192000
	6	0.550004000	0.774161000	-0.202923000
	6	-1.895775000	0.538176000	-0.016337000
	1	-2.876755000	0.990802000	0.029077000
	6	0.629680000	-0.645967000	-0.119862000
	6	-1.739179000	-0.830036000	0.056034000
	6	-0.491607000	-1.437887000	0.009848000
TS7	1	-0.413312000	-2.515741000	0.060628000
	7	-0.998621000	2.776307000	-0.171071000
	8	-0.083809000	3.502160000	-0.522072000
	8	-2.092355000	3.170903000	0.148932000
	7	1.687274000	1.491542000	-0.383673000
	1	1.533062000	2.494298000	-0.423973000
	1	2.591163000	1.205198000	0.233458000
	35	2.307258000	-1.482969000	-0.240936000
	7	-2.940706000	-1.678002000	0.171916000
	8	-2.767700000	-2.874658000	0.230141000
	8	-4.012784000	-1.117997000	0.201531000
	8	3.128151000	1.216551000	1.424976000
	1	3.055975000	2.110665000	1.789909000
	6	-1.643614000	-0.590205000	-0.000012000
	6	-0.413961000	-1.305833000	0.000048000
	6	-1.707523000	0.795325000	-0.000009000
	1	-2.669749000	1.290306000	-0.000044000
	6	0.760951000	-0.488216000	-0.000023000
	6	-0.541665000	1.528855000	-0.000013000
	6	0.684474000	0.871744000	0.000019000

TS8	1	1.799049000	1.476067000	0.000027000
	7	-2.932107000	-1.289358000	-0.000032000
	8	-2.923240000	-2.510742000	0.000041000
	8	-3.939293000	-0.623774000	-0.000054000
	7	-0.304333000	-2.638549000	0.000081000
	1	-1.134413000	-3.210255000	0.000273000
	1	0.613291000	-3.054376000	0.000255000
	35	2.458476000	-1.323370000	-0.000041000
	7	-0.625551000	2.991307000	-0.000006000
	8	0.417160000	3.617558000	0.000101000
	8	-1.726799000	3.487958000	-0.000060000
	8	2.812357000	2.093583000	0.000044000
	1	2.425657000	2.985719000	0.000006000
	6	-0.774385000	1.106704000	-0.031799000
	6	0.650697000	1.088188000	0.008809000
TS9	6	-1.520613000	-0.064119000	-0.051814000
	1	-2.814056000	-0.094731000	0.014249000
	6	1.244047000	-0.209165000	-0.006363000
	6	-0.890621000	-1.281234000	-0.040536000
	6	0.503827000	-1.360768000	-0.026588000
	1	0.976824000	-2.334658000	-0.023780000
	7	-1.489260000	2.381362000	-0.087216000
	8	-2.653820000	2.373414000	-0.421694000
	8	-0.881001000	3.398619000	0.194847000
	7	1.426686000	2.181516000	0.031452000
	1	1.013084000	3.093279000	0.137008000
	1	2.427650000	2.070638000	0.043815000
	35	3.132392000	-0.349313000	0.006551000
	7	-1.658932000	-2.535201000	-0.053871000
	8	-1.038614000	-3.560899000	0.135321000
	8	-2.845093000	-2.455943000	-0.261090000
	8	-3.888681000	0.070284000	0.473527000
	1	-4.006714000	1.016241000	0.289306000
	6	2.202746000	-0.464490000	-0.007678000
	6	1.095746000	-1.358789000	0.068015000
	6	2.013664000	0.906088000	-0.020828000
	1	2.864349000	1.572079000	-0.077895000
	6	-0.248541000	-0.775503000	0.137011000
	6	0.711269000	1.426074000	0.043728000
	6	-0.412371000	0.630334000	0.123197000
	1	-1.410024000	1.054770000	0.163833000
	7	3.577570000	-0.957896000	-0.077115000
	8	3.755488000	-2.186264000	-0.071403000
	8	4.482769000	-0.136400000	-0.137126000
	7	1.164995000	-2.686792000	0.081360000
	1	2.072284000	-3.137377000	0.031829000
	1	0.294799000	-3.205290000	0.135372000
	35	-3.852138000	-0.447203000	-0.091059000
	7	0.552140000	2.893476000	0.032214000
	8	-0.589290000	3.334755000	0.104537000

TS10	8	1.578440000	3.566443000	-0.048761000
	8	-1.219372000	-1.627083000	0.213573000
	1	-2.298873000	-1.167485000	0.131494000
TS11	6	0.069650000	1.278249000	-0.375390000
	6	0.932624000	0.595460000	0.580620000
	6	-1.184855000	0.845530000	-0.592408000
	1	-1.886109000	1.431556000	-1.171564000
	6	0.694874000	-0.902508000	0.667590000
	6	-1.577636000	-0.444700000	-0.077937000
	6	-0.732995000	-1.288517000	0.514426000
	1	-1.055080000	-2.266737000	0.851434000
	7	0.403428000	2.620487000	-0.863819000
	8	1.298515000	3.216190000	-0.293332000
	8	-0.232059000	3.051350000	-1.793461000
	7	2.202197000	0.959041000	0.840245000
	1	2.424004000	1.942576000	0.814266000
	1	2.705113000	0.373436000	1.491336000
	35	1.618282000	-1.766496000	-0.935418000
	7	-2.991496000	-0.849511000	-0.246384000
	8	-3.317290000	-1.928194000	0.191204000
	8	-3.715998000	-0.065460000	-0.813328000
	8	1.303477000	-1.355659000	1.810100000
	1	1.247891000	-2.316275000	1.861053000
	8	0.015507000	1.052358000	2.143131000
	8	-1.175219000	1.410865000	2.065864000
	6	1.245511000	1.010766000	0.111546000
	6	1.258971000	-0.308607000	0.562825000
	6	0.062080000	1.633391000	-0.344830000
	1	0.112853000	2.642285000	-0.733641000
	6	-0.020483000	-1.097053000	0.416923000
	6	-1.133081000	0.981769000	-0.266817000
	6	-1.251006000	-0.292105000	0.322717000
	1	-2.194632000	-0.822027000	0.268867000
	7	2.457139000	1.802904000	0.103056000
	8	3.482733000	1.283872000	0.530021000
	8	2.399958000	2.933115000	-0.322084000
	7	2.273950000	-0.980830000	1.070400000
	1	3.179013000	-0.535265000	1.140787000
	1	2.121571000	-1.931265000	1.377102000
	35	0.170678000	-1.947712000	-1.491436000
	7	-2.360072000	1.671940000	-0.665139000
	8	-3.404630000	1.082206000	-0.477451000
	8	-2.255397000	2.773517000	-1.154953000
	8	-0.018639000	-2.112981000	1.323813000
TS12	1	-0.874217000	-2.557250000	1.351871000
	8	-1.480715000	0.132995000	2.263672000
	8	-1.959233000	-0.799426000	2.889839000
	6	-0.562619000	1.222175000	-0.337909000
	6	0.616170000	1.090923000	0.384863000

TS13	6	-1.486661000	0.152939000	-0.472189000
	1	-2.346996000	0.277907000	-1.113640000
	6	1.105623000	-0.306585000	0.695452000
	6	-1.010237000	-1.165056000	-0.178751000
	6	0.129855000	-1.398090000	0.477182000
	1	0.403986000	-2.399975000	0.786366000
	7	-1.051008000	2.530091000	-0.720762000
	8	-0.331689000	3.499333000	-0.508001000
	8	-2.138321000	2.601101000	-1.246014000
	7	1.421595000	2.055719000	0.798951000
	1	1.195674000	3.017645000	0.587712000
	1	2.228818000	1.810783000	1.353237000
	35	2.568573000	-0.679019000	-0.706161000
	7	-1.934411000	-2.294863000	-0.420178000
	8	-1.553562000	-3.400606000	-0.109891000
	8	-3.003581000	-2.027974000	-0.916139000
	8	1.709185000	-0.288286000	1.927164000
	1	2.086396000	-1.152566000	2.127231000
	8	-2.459777000	0.335518000	1.221448000
	8	-1.631500000	0.355590000	2.126028000
TS14	6	1.478050000	0.254636000	-0.166023000
	6	0.959647000	-1.061705000	-0.013991000
	6	0.545187000	1.320844000	-0.577006000
	1	0.800415000	2.040149000	-1.343879000
	6	-0.413540000	-1.084422000	0.590579000
	6	-0.576564000	1.321295000	0.132131000
	6	-0.650795000	0.306099000	1.216142000
	1	-1.575604000	0.345663000	1.789713000
	7	2.863526000	0.441380000	-0.640066000
	8	3.585475000	-0.537401000	-0.702826000
	8	3.193104000	1.569328000	-0.904002000
	7	1.607198000	-2.216868000	-0.110889000
	1	2.579865000	-2.230912000	-0.381872000
	1	1.159512000	-3.043991000	0.258660000
	35	-1.819939000	-1.395799000	-0.837654000
	7	-1.643265000	2.289013000	-0.085266000
	8	-2.588886000	2.236742000	0.673089000
	8	-1.513496000	3.064284000	-1.004397000
	8	-0.462401000	-2.124089000	1.482682000
	1	-1.344780000	-2.190655000	1.865780000
	8	0.420787000	0.481352000	2.157014000
	8	1.644711000	0.809475000	1.534949000
	6	1.163652000	0.870822000	-0.158118000
	6	1.239793000	-0.429628000	0.489860000
	6	-0.069462000	1.498862000	-0.374104000
	1	-0.104057000	2.435142000	-0.916876000
	6	-0.069292000	-1.227143000	0.504465000
	6	-1.203146000	0.941910000	0.129053000

TS15	6	-1.109099000	-0.240333000	1.020740000
	1	-2.071079000	-0.686458000	1.263361000
	7	2.356062000	1.586228000	-0.543553000
	8	3.440950000	1.113649000	-0.227466000
	8	2.222691000	2.619136000	-1.161814000
	7	2.345783000	-1.159269000	0.567008000
	1	3.239899000	-0.696955000	0.484418000
	1	2.271326000	-2.066668000	1.003774000
	35	-0.534817000	-1.814308000	-1.310750000
	7	-2.485975000	1.593680000	-0.037569000
	8	-3.436417000	1.090053000	0.533376000
	8	-2.534655000	2.578811000	-0.741541000
	8	0.125985000	-2.307554000	1.331224000
	1	-0.675642000	-2.839942000	1.381684000
	8	-0.535180000	0.273020000	2.248401000
	8	0.820673000	0.223418000	2.153733000
	6	1.216192000	0.951001000	-0.073297000
	6	1.403321000	-0.311008000	0.495434000
	6	-0.062153000	1.457455000	-0.394603000
	1	-0.146058000	2.361143000	-0.983818000
	6	0.169221000	-1.186385000	0.654937000
	6	-1.190186000	0.863623000	0.120741000
	6	-1.078378000	-0.381365000	0.969866000
	1	-1.976028000	-1.003091000	0.927770000
	7	2.356142000	1.771067000	-0.429354000
	8	3.474175000	1.355198000	-0.142361000
	8	2.151026000	2.821687000	-0.989647000
	7	2.537099000	-0.872900000	0.857606000
	1	3.404313000	-0.366382000	0.731054000
	1	2.508273000	-1.788096000	1.285495000
	35	-0.140936000	-2.029456000	-1.133366000
	7	-2.495494000	1.207162000	-0.471549000
	8	-3.381552000	0.391549000	-0.350115000
	8	-2.584812000	2.278878000	-1.021581000
	8	0.445199000	-2.144029000	1.596487000
	1	-0.326473000	-2.702146000	1.746745000
	8	-0.896115000	0.236221000	2.230066000
	8	-1.465869000	1.489532000	1.880299000
TS16	6	1.148489000	1.094779000	-0.016334000
	6	1.390353000	-0.150644000	0.540563000
	6	-0.156215000	1.475941000	-0.465215000
	1	-0.263019000	2.390162000	-1.036855000
	6	0.226463000	-1.141810000	0.576729000
	6	-1.230088000	0.724722000	-0.187503000
	6	-1.142017000	-0.475208000	0.675163000
	1	-1.932810000	-1.196500000	0.466157000
	7	2.215902000	2.042506000	-0.204514000

TS17	8	3.341156000	1.721402000	0.168248000
	8	1.955368000	3.108453000	-0.715958000
	7	2.525498000	-0.625118000	1.014456000
	1	3.357909000	-0.051820000	0.969436000
	1	2.527780000	-1.542996000	1.436508000
	35	0.278291000	-2.048657000	-1.194132000
	7	-2.550139000	1.109517000	-0.665173000
	8	-3.465277000	0.350740000	-0.410514000
	8	-2.651373000	2.143116000	-1.287162000
	8	0.451541000	-2.075880000	1.561839000
	1	-0.304666000	-2.144428000	2.156454000
	8	-1.251767000	-0.130902000	2.103366000
	8	-2.115413000	0.807269000	2.336320000
	6	1.749179000	-0.644995000	0.002348000
	6	0.527020000	-1.259620000	0.240208000
	6	1.871293000	0.765945000	-0.186889000
	1	2.856641000	1.179247000	-0.367299000
	6	-0.677630000	-0.382054000	0.093348000
	6	0.802344000	1.576629000	-0.121624000
	6	-0.533050000	1.059769000	0.184213000
	1	-1.406279000	1.671317000	-0.031523000
	7	2.973641000	-1.414366000	0.022829000
	8	2.889043000	-2.612084000	0.269931000
	8	4.012160000	-0.843127000	-0.213262000
	7	0.286130000	-2.520698000	0.544928000
	1	1.064477000	-3.159874000	0.645890000
	1	-0.660299000	-2.807849000	0.754160000
	35	-2.100923000	-1.155605000	-0.904606000
	7	0.954705000	3.018738000	-0.274975000
	8	-0.043719000	3.688556000	-0.111327000
	8	2.052510000	3.442658000	-0.557291000
	8	-3.623208000	1.386974000	0.525438000
	1	-3.178771000	0.896825000	1.257272000
	8	-0.571891000	0.485350000	1.556494000
	8	-1.849859000	-0.249982000	1.790470000
TS18	6	1.483732000	0.681236000	0.157974000
	6	1.267548000	-0.659748000	0.439645000
	6	0.407272000	1.574194000	-0.111330000
	1	0.638588000	2.563282000	-0.490058000
	6	-0.158357000	-1.220539000	0.332909000
	6	-0.876723000	1.225730000	0.072921000
	6	-1.299411000	-0.060542000	0.664293000
	1	-2.239006000	-0.469829000	0.296055000
	7	2.819439000	1.222945000	0.109211000
	8	3.752288000	0.465391000	0.357957000
	8	2.956298000	2.392512000	-0.169649000
	7	2.151397000	-1.573321000	0.780146000

TS19	1	3.131489000	-1.325983000	0.832677000
	1	1.818021000	-2.503550000	0.997020000
	35	-0.458466000	-1.546975000	-1.64384300
	7	-1.945932000	2.148688000	-0.284873000
	8	-3.081061000	1.762409000	-0.079920000
	8	-1.643610000	3.223696000	-0.749906000
	8	-0.376379000	-2.264959000	1.044262000
	1	-1.303809000	-1.862114000	2.047608000
	8	-1.304827000	0.028966000	2.047840000
	8	-1.817418000	-1.118996000	2.584582000
	6	-1.475856000	1.060430000	-0.280103000
	6	-1.491591000	-0.235544000	-0.774415000
	6	-0.408923000	1.526703000	0.547850000
	1	-0.533797000	2.462272000	1.080170000
	6	-0.344474000	-1.168191000	-0.369013000
	6	0.719125000	0.813897000	0.693183000
	6	0.965626000	-0.414472000	-0.097777000
	1	1.717079000	-1.075821000	0.331300000
	7	-2.570633000	1.961957000	-0.522266000
	8	-3.509436000	1.555954000	-1.201834000
	8	-2.512503000	3.076242000	-0.051604000
	7	-2.401212000	-0.804032000	-1.537272000
	1	-3.222947000	-0.278336000	-1.805826000
	1	-2.234981000	-1.749794000	-1.854458000
	35	-0.889802000	-1.910483000	1.395716000
TS20	7	1.737659000	1.232142000	1.647406000
	8	2.628038000	0.439492000	1.884410000
	8	1.620676000	2.323905000	2.157834000
	8	-0.234647000	-2.201730000	-1.257025000
	1	0.631082000	-2.156341000	-1.707994000
	8	1.461397000	0.002258000	-1.420510000
	8	2.004538000	-1.032069000	-2.074778000
	1	3.546996000	-0.553685000	-1.919444000
	8	3.767578000	0.444329000	-1.891775000
	8	3.036297000	0.890518000	-0.945623000
	6	-1.030287000	1.069841000	-0.200880000
	6	0.432381000	1.022978000	-0.282342000
	6	-1.772023000	0.057893000	0.248755000
	1	-2.833400000	0.185461000	0.421647000
	6	0.997498000	-0.324097000	-0.098665000
	6	-1.201762000	-1.293558000	0.486379000
	6	0.285089000	-1.363163000	0.333816000
	1	0.751349000	-2.315901000	0.558233000
	7	-1.735633000	2.359663000	-0.393470000
	8	-1.057636000	3.365044000	-0.481965000
	8	-2.938568000	2.335800000	-0.443091000
	7	1.136421000	1.930687000	-0.989179000
	1	0.780820000	2.874938000	-1.015776000
	1	2.136969000	1.808292000	-1.027727000
	35	2.872604000	-0.502672000	-0.279863000

TS21	7	-1.744628000	-2.244696000	-0.673634000
	8	-1.851499000	-3.409389000	-0.366211000
	8	-1.942397000	-1.763233000	-1.755349000
	8	-1.687565000	-1.804852000	1.663333000
	1	-1.557814000	-2.763840000	1.663480000
	8	0.683688000	1.532725000	1.585634000
	8	0.084281000	0.802111000	2.381015000
	6	1.588455000	-0.583585000	0.189570000
	6	0.329798000	-1.298369000	-0.063839000
	6	1.686384000	0.746401000	0.231212000
	1	2.630423000	1.236499000	0.430567000
	6	-0.813671000	-0.503918000	-0.082888000
	6	0.496291000	1.602786000	-0.010918000
	6	-0.796701000	0.868809000	0.174897000
	1	-1.694195000	1.451650000	-0.003087000
	7	2.856625000	-1.325822000	0.407775000
	8	2.938437000	-2.450596000	-0.048720000
	8	3.737158000	-0.760412000	1.001376000
	7	0.288662000	-2.631651000	-0.213009000
	1	1.142405000	-3.155994000	-0.318564000
	1	-0.601386000	-3.072462000	-0.385308000
	35	-2.503529000	-1.336365000	-0.273343000
	7	0.479792000	1.985620000	-1.577270000
	8	-0.207183000	2.937919000	-1.847389000
	8	1.091550000	1.289583000	-2.344981000
	8	0.642418000	2.778950000	0.667640000
	1	-0.191524000	3.264792000	0.691130000
	8	-1.003975000	1.042604000	2.139664000
	8	-1.446044000	2.144265000	2.457606000
TS22	6	1.023289000	-0.976549000	-0.249933000
	6	-0.367019000	-1.028231000	-0.427294000
	6	1.633310000	0.098628000	0.396040000
	1	2.701080000	0.081774000	0.564529000
	6	-1.110754000	0.192086000	-0.040488000
	6	0.982277000	1.432625000	0.370152000
	6	-0.514562000	1.327041000	0.320761000
	1	-1.082099000	2.207130000	0.598562000
	7	1.840762000	-2.157062000	-0.449277000
	8	1.337756000	-3.125059000	-1.008892000
	8	2.988749000	-2.125257000	-0.069915000
	7	-1.043608000	-2.045518000	-0.946776000
	1	-0.538781000	-2.882576000	-1.205719000
	1	-2.049973000	-2.009309000	-0.992325000
	35	-3.002952000	0.112547000	-0.046766000
	7	1.362631000	2.182451000	-1.001968000
	8	1.533522000	3.376634000	-0.903542000
	8	1.384102000	1.536509000	-2.012004000
	8	1.454828000	2.225891000	1.383645000
	1	1.392643000	3.151415000	1.104495000
	8	1.078333000	-0.316892000	2.320227000

TS25	6	-0.949577000	0.951571000	0.275040000
	6	0.309658000	1.049531000	-0.261768000
	6	-1.248085000	-0.291317000	1.018701000
	1	-2.271445000	-0.326231000	1.388937000
	6	1.120275000	-0.195700000	-0.020558000
	6	-0.921820000	-1.511831000	0.103713000
	6	0.527131000	-1.431491000	-0.223487000
	1	1.101042000	-2.345316000	-0.285643000
	7	-1.894838000	2.009970000	0.228906000
	8	-1.580189000	3.029931000	-0.380714000
	8	-2.965612000	1.855217000	0.782154000
	7	0.842328000	2.064856000	-0.926315000
	1	0.273459000	2.888978000	-1.075192000
	1	1.797805000	2.021158000	-1.244065000
	35	2.994592000	-0.059283000	-0.199788000
	7	-1.823901000	-1.342274000	-1.165705000
	8	-2.981493000	-1.642546000	-0.988037000
	8	-1.337113000	-0.918757000	-2.180391000
	8	-1.204008000	-2.733755000	0.650160000
	1	-2.150311000	-2.785845000	0.840508000
	8	-0.388452000	-0.477904000	2.155857000
	8	0.900382000	-0.103472000	1.843472000
TS26	6	-1.088036000	0.930508000	0.157112000
	6	0.248637000	1.131852000	-0.186796000
	6	-1.518597000	-0.356223000	0.770068000
	1	-2.599339000	-0.453882000	0.827315000
	6	1.124738000	-0.023705000	-0.000897000
	6	-0.851985000	-1.524417000	0.057402000
	6	0.625328000	-1.270719000	0.267984000
	1	1.279683000	-2.132810000	0.303740000
	7	-2.055514000	1.981717000	0.110391000
	8	-1.724619000	3.057653000	-0.382927000
	8	-3.164010000	1.759477000	0.553436000
	7	0.767760000	2.271295000	-0.639452000
	1	0.157301000	3.066141000	-0.769134000
	1	1.750567000	2.325753000	-0.853684000
	35	2.986778000	0.225250000	-0.046643000
	7	-1.221119000	-1.492388000	-1.428414000
	8	-0.336533000	-1.706940000	-2.220125000
	8	-2.381301000	-1.288668000	-1.676575000
	8	-1.270137000	-2.770237000	0.471094000
	1	-0.986469000	-2.877242000	1.389073000
	8	-0.965084000	-0.386581000	2.113579000
	8	0.114510000	-1.222184000	2.147556000
	6	-0.720482000	1.321926000	-0.282101000
	6	0.641339000	1.130848000	-0.165796000
	6	-1.734749000	0.230328000	-0.262268000
	1	-2.493132000	0.349136000	-1.035512000

TS27	6	1.121838000	-0.274838000	-0.203241000
	6	-1.087988000	-1.136661000	-0.222118000
	6	0.283044000	-1.350973000	-0.314749000
	1	0.660582000	-2.362051000	-0.383973000
	7	-1.295917000	2.630512000	-0.346067000
	8	-0.559106000	3.612092000	-0.290187000
	8	-2.502908000	2.704391000	-0.465668000
	7	1.558159000	2.095241000	-0.090492000
	1	1.242968000	3.054335000	-0.041132000
	1	2.522984000	1.857768000	0.073928000
	35	2.964698000	-0.593475000	-0.285666000
	7	-1.974870000	-2.281431000	-0.496823000
	8	-1.507611000	-3.388192000	-0.343352000
	8	-3.105701000	-2.019579000	-0.836176000
	8	1.086380000	-0.162378000	2.285072000
	1	0.165563000	-0.224722000	2.601862000
	8	-2.427698000	0.148924000	1.003124000
	8	-1.594986000	-0.712368000	1.649495000
	6	-1.675611000	-0.392345000	-0.072753000
	6	-0.455210000	-1.232976000	0.039025000
	6	-1.661119000	0.932801000	-0.016577000
	1	-2.578068000	1.506570000	-0.066796000
	6	0.734538000	-0.604991000	-0.159365000
	6	-0.374322000	1.707514000	0.029312000
	6	0.862025000	0.796561000	-0.588446000
	1	1.761795000	1.311112000	-0.243786000
	7	-3.007230000	-1.031479000	-0.238381000
	8	-3.025457000	-2.183086000	-0.628278000
	8	-3.981434000	-0.365597000	-0.002379000
	7	-0.567351000	-2.509292000	0.473905000
	1	-1.433927000	-2.998234000	0.313547000
	1	0.274683000	-3.063943000	0.505895000
	35	2.360617000	-1.519028000	0.116884000
	7	0.097851000	1.849350000	1.548719000
	8	1.118199000	2.456475000	1.720901000
	8	-0.613866000	1.357377000	2.386545000
	8	-0.407466000	2.863421000	-0.549234000
	1	0.406462000	2.772765000	-1.605981000
	8	0.735999000	0.929884000	-1.966277000
	8	1.011870000	2.221313000	-2.320115000
TS28	6	0.171195000	1.504813000	-0.456621000
	6	-1.112086000	1.014886000	-0.366340000
	6	1.387925000	0.730238000	-0.071999000
	1	2.147961000	1.412021000	0.316907000
	6	-1.271485000	-0.333573000	0.250366000
	6	1.067651000	-0.342603000	0.997191000
	6	-0.286460000	-0.956578000	0.881502000
	1	-0.410421000	-1.935655000	1.327745000

TS29	7	0.444025000	2.786667000	-1.028627000
	8	-0.496567000	3.472565000	-1.426863000
	8	1.601999000	3.151079000	-1.087593000
	7	-2.218887000	1.644889000	-0.754260000
	1	-2.128658000	2.561829000	-1.172135000
	1	-3.118579000	1.208283000	-0.634138000
	35	-2.952812000	-1.185719000	0.108963000
	7	1.172595000	0.424458000	2.357738000
	8	2.265047000	0.393864000	2.876855000
	8	0.207486000	1.024910000	2.742423000
	8	2.004467000	-1.358453000	1.027904000
	1	2.837703000	-1.010751000	1.382566000
	8	2.040290000	0.142917000	-1.194014000
	8	1.323940000	-0.932447000	-1.653442000
	8	1.883518000	-3.601240000	-1.813418000
	8	2.488221000	-2.589850000	-1.436512000
	1	1.948663000	-2.057507000	-0.745912000
	6	1.475486000	-0.751117000	-0.095283000
	6	0.166645000	-1.129401000	-0.310386000
	6	1.833184000	0.513524000	0.621384000
	1	2.862824000	0.815738000	0.442807000
	6	-0.852382000	-0.227045000	0.250455000
	6	0.816099000	1.625336000	0.372249000
	6	-0.361685000	0.932874000	1.085096000
	1	-1.169503000	1.610428000	1.362944000
	7	2.572952000	-1.563252000	-0.522245000
	8	2.328006000	-2.610799000	-1.114135000
	8	3.700356000	-1.175962000	-0.285439000
	7	-0.261552000	-2.219930000	-0.954513000
	1	0.418650000	-2.862528000	-1.334255000
	1	-1.249265000	-2.389880000	-1.054976000
	35	-2.424290000	0.038713000	-0.721574000
	7	0.477120000	1.938765000	-1.089407000
	8	-0.381042000	2.786231000	-1.213083000
	8	1.068398000	1.384987000	-1.977003000
	8	1.230651000	2.790088000	0.955531000
	1	0.517964000	3.440939000	0.919550000
	8	1.685274000	0.378748000	2.029176000
	8	0.256705000	0.458091000	2.267617000
	8	-1.548524000	-1.469663000	1.739319000
	8	-2.654105000	-1.897190000	1.515654000
	6	1.847719000	-0.807515000	0.184378000
	6	0.600482000	-1.289815000	-0.099417000
	6	2.064996000	0.496129000	0.888951000
	1	3.104603000	0.814374000	0.856204000
TS30	6	-0.579553000	-0.398097000	0.257218000
	6	1.085334000	1.566419000	0.423719000
	6	-0.180654000	0.896905000	0.992292000
	1	-1.034252000	1.566869000	1.085197000
	7	3.025075000	-1.559110000	-0.140877000
	8	2.884722000	-2.661134000	-0.662139000
	8	4.107792000	-1.068820000	0.106975000
	7	0.273650000	-2.460758000	-0.647087000
	1	1.008792000	-3.094065000	-0.927255000

TS31	1	-0.692916000	-2.666938000	-0.841927000
	35	-1.568532000	0.083641000	-1.399504000
	7	1.053821000	1.844901000	-1.086024000
	8	0.373380000	2.798863000	-1.388575000
	8	1.702717000	1.163876000	-1.833939000
	8	1.364984000	2.756634000	1.040411000
	1	0.712417000	3.414606000	0.766673000
	8	1.700970000	0.415396000	2.260492000
	8	0.253847000	0.551245000	2.289372000
	8	-1.407912000	-1.190190000	1.058684000
	8	-2.430569000	-0.459018000	1.567654000
	1	-3.815103000	-1.248633000	1.416401000
	8	-4.072529000	-0.914615000	0.500112000
	8	-4.962738000	-0.051367000	0.543755000
	6	1.809767000	-0.813193000	0.214502000
	6	0.552638000	-1.321455000	0.036399000
	6	2.062404000	0.531743000	0.823070000
	1	3.101116000	0.838501000	0.721979000
	6	-0.618264000	-0.407244000	0.429785000
	6	1.070421000	1.576561000	0.330455000
	6	-0.169552000	0.959033000	1.007253000
	1	-1.017664000	1.640559000	1.079332000
	7	2.970009000	-1.579516000	-0.142025000
	8	2.803153000	-2.704288000	-0.601600000
	8	4.063168000	-1.077034000	0.020981000
	7	0.194251000	-2.522719000	-0.411095000
	1	0.909317000	-3.171774000	-0.705945000
	1	-0.784592000	-2.753838000	-0.476343000
	35	-1.644044000	0.000056000	-1.340107000
	7	0.976282000	1.752076000	-1.190198000
	8	0.289680000	2.690533000	-1.527215000
	8	1.590009000	1.017814000	-1.916275000
	8	1.386238000	2.804544000	0.851151000
	1	0.745131000	3.454386000	0.533445000
	8	1.761805000	0.546349000	2.213764000
	8	0.322375000	0.725010000	2.305202000
	8	-1.398286000	-1.092146000	1.236152000
	8	-3.014802000	-0.158299000	1.493736000
	7	-3.727052000	-0.659618000	0.692298000
	8	-4.872173000	-0.514236000	0.431558000
TS32	6	-1.275344000	-0.743730000	-0.543632000
	6	-0.487651000	0.239265000	-1.090009000
	6	-1.136711000	-1.166087000	0.878691000
	1	-1.672819000	-2.087407000	1.097229000
	6	0.468940000	0.977890000	-0.137716000
	6	0.317591000	-1.182062000	1.338254000
	6	0.554793000	0.326577000	1.262114000
	1	1.422379000	0.685808000	1.813694000
	7	-2.288291000	-1.406464000	-1.304940000
	8	-2.438478000	-1.080637000	-2.477937000
	8	-2.956461000	-2.263280000	-0.756921000

TS33	7	-0.530094000	0.727719000	-2.320725000
	1	-1.185372000	0.347704000	-2.988375000
	1	0.089672000	1.486607000	-2.562927000
	35	2.338198000	0.845421000	-0.925060000
	7	1.304266000	-1.980927000	0.469202000
	8	2.413181000	-2.043428000	0.950118000
	8	0.934154000	-2.496164000	-0.549745000
	8	0.404249000	-1.684660000	2.610809000
	1	1.327412000	-1.657087000	2.896694000
	8	-1.668262000	-0.183580000	1.792639000
	8	-0.616664000	0.811314000	1.942223000
	8	0.115341000	2.240431000	0.001614000
	1	-1.042609000	2.012849000	1.116130000
	8	-1.892260000	2.632085000	0.712499000
	8	-1.898112000	3.758965000	1.131412000
	6	-0.686491000	1.419576000	0.144726000
	6	0.664619000	0.724721000	0.160284000
	6	-1.834645000	0.476877000	0.266925000
	1	-2.812499000	0.889045000	0.481566000
	6	0.728980000	-0.672424000	-0.234012000
	6	-1.642107000	-0.827911000	0.077857000
	6	-0.372919000	-1.442306000	-0.244814000
	1	-0.339374000	-2.500216000	-0.460566000
	7	-0.775664000	2.116928000	-1.272374000
	8	-0.291618000	3.210533000	-1.369305000
	8	-1.264651000	1.455258000	-2.153451000
	7	1.713573000	1.537252000	0.095005000
	1	1.590625000	2.506985000	0.357163000
	1	2.649329000	1.158131000	0.097781000
	35	2.433334000	-1.418794000	-0.527392000
	7	-2.819055000	-1.730538000	0.185983000
	8	-2.641375000	-2.891615000	-0.103345000
	8	-3.863536000	-1.245669000	0.549946000
	8	-0.731891000	2.487261000	1.022936000
	1	-0.650942000	2.138730000	1.920361000
	8	0.578693000	0.293823000	2.149202000
	8	1.516825000	0.931463000	2.651058000
	6	1.709979000	-0.201777000	0.549884000
	6	0.567527000	-1.163114000	0.282374000
	6	1.419095000	1.232772000	0.269506000
	1	2.207905000	1.952522000	0.447413000
	6	-0.619661000	-0.687338000	-0.171490000
	6	0.214286000	1.601675000	-0.160910000
	6	-0.900070000	0.704540000	-0.335044000
	1	-1.716526000	1.012635000	-0.974592000
	7	2.855967000	-0.647845000	-0.465292000
	8	3.476217000	-1.637642000	-0.145733000
	8	2.996735000	-0.009326000	-1.472403000
	7	0.827575000	-2.462282000	0.634361000
	1	1.757386000	-2.814364000	0.435427000

TS34	1	0.083314000	-3.124280000	0.462728000
	35	-2.055554000	-1.884474000	-0.466860000
	7	-0.047896000	3.043246000	-0.393554000
	8	-1.161396000	3.336473000	-0.765329000
	8	0.859958000	3.815513000	-0.198793000
	8	2.234727000	-0.317861000	1.811920000
	1	2.155238000	-1.230058000	2.118856000
	8	-1.883811000	1.143959000	1.282740000
	8	-3.064852000	1.382353000	1.089564000
TS36	6	0.722037000	-1.255620000	0.036773000
	6	-0.748719000	-0.993782000	0.250790000
	6	1.582848000	-0.035388000	0.125062000
	1	2.651246000	-0.178911000	0.009072000
	6	-1.226259000	0.276773000	0.058391000
	6	0.988817000	1.178145000	-0.262423000
	6	-0.371489000	1.356308000	-0.251476000
	1	-0.781129000	2.337110000	-0.457061000
	7	0.883653000	-1.736484000	-1.496912000
	8	0.140398000	-1.283532000	-2.320797000
	8	1.816849000	-2.482423000	-1.683091000
	7	-1.479352000	-2.081974000	0.522388000
	1	-1.005459000	-2.928672000	0.799298000
	1	-2.472531000	-1.997717000	0.677217000
	35	-3.087504000	0.584791000	0.180359000
	7	1.859047000	2.330627000	-0.488626000
	8	1.338391000	3.384398000	-0.784203000
	8	3.053530000	2.149476000	-0.368683000
	8	1.114514000	-2.320598000	0.804605000
	1	1.981752000	-2.629347000	0.506365000
	8	1.656793000	0.131382000	2.086088000
	8	2.524763000	-0.555444000	2.597567000
	6	0.735622000	-1.389146000	0.130357000
	6	-0.721774000	-0.987531000	0.297752000
	6	1.569913000	-0.259980000	0.732432000
	1	2.637204000	-0.474239000	0.745880000
	6	-1.064198000	0.349563000	-0.031666000
	6	1.232186000	1.022625000	0.054620000
	6	-0.069511000	1.318510000	-0.225530000
	1	-0.330232000	2.312026000	-0.570104000
	7	1.113854000	-1.497156000	-1.373525000
	8	0.350914000	-1.108761000	-2.213623000
	8	2.200162000	-1.999952000	-1.554173000
	7	-1.598306000	-1.984907000	0.347355000
	1	-1.266524000	-2.887042000	0.658768000
	1	-2.581669000	-1.774091000	0.431105000
	35	-2.876920000	0.804132000	-0.208101000
	7	2.257469000	2.033209000	-0.071330000
	8	1.947422000	3.102354000	-0.556420000
	8	3.375533000	1.736138000	0.309639000
	8	0.933862000	-2.622481000	0.690884000

TS37	1	1.851710000	-2.891990000	0.554154000
	8	1.113826000	-0.131479000	2.087306000
	8	-0.187073000	-0.552265000	2.161193000
	6	-0.787674000	1.343743000	0.285694000
	6	0.653327000	1.140469000	-0.081899000
	6	-1.271781000	0.061501000	1.009584000
	1	-2.293106000	0.172639000	1.372612000
	6	1.083550000	-0.194909000	-0.037183000
	6	-1.090321000	-1.091652000	0.086281000
	6	0.132155000	-1.252734000	-0.414256000
	1	0.431852000	-2.105090000	-1.010734000
	7	-1.682963000	1.516674000	-0.990022000
	8	-1.255305000	1.171573000	-2.058165000
	8	-2.781336000	1.970318000	-0.759428000
	7	1.432754000	2.222780000	-0.183370000
	1	1.071867000	3.107442000	0.145379000
	1	2.431357000	2.112806000	-0.279520000
	35	2.912054000	-0.555420000	-0.321549000
	7	-2.154796000	-2.061530000	-0.137768000
	8	-1.909580000	-3.005716000	-0.853558000
TS38	8	-3.216219000	-1.841189000	0.407270000
	8	-0.912041000	2.494170000	1.021605000
	1	-1.849310000	2.665922000	1.186668000
	8	-0.440991000	-0.079600000	2.160359000
	8	0.866090000	-0.496806000	1.822996000
	6	-0.746140000	1.389506000	0.393032000
	6	0.730413000	1.105799000	0.165097000
	6	-1.474262000	0.110604000	0.829420000
	1	-2.542992000	0.269939000	0.982243000
	6	1.141032000	-0.174015000	-0.071746000
	6	-1.148001000	-0.994658000	-0.123958000
	6	0.225849000	-1.266490000	-0.135267000
	1	0.563336000	-2.245820000	-0.452371000
	7	-1.402344000	1.832984000	-0.957618000
	8	-1.019517000	1.311795000	-1.969644000
	8	-2.306602000	2.629194000	-0.845975000
	7	1.512649000	2.193524000	0.195684000
	1	1.146642000	3.033806000	0.618477000
	1	2.513391000	2.085728000	0.123287000
	35	2.982445000	-0.533841000	-0.273828000
	7	-2.116349000	-2.011873000	-0.431127000
	8	-1.709867000	-3.043421000	-0.923475000
	8	-3.280797000	-1.744122000	-0.199414000
	8	-0.873782000	2.425098000	1.280697000
	1	-1.768431000	2.789153000	1.207762000
	8	-0.811201000	-0.288041000	2.031865000
	8	-0.326801000	-1.587417000	1.765511000

TS39	6	-0.601448000	1.442057000	0.334860000
	6	0.851671000	1.017911000	0.315040000
	6	-1.544349000	0.291800000	0.688798000
	1	-2.584168000	0.551792000	0.468031000
	6	1.161481000	-0.284026000	-0.001618000
	6	-1.130367000	-1.029412000	0.078458000
	6	0.180898000	-1.265109000	-0.255524000
	1	0.457331000	-2.230666000	-0.659033000
	7	-1.013843000	1.890315000	-1.116052000
	8	-0.573209000	1.276825000	-2.049025000
	8	-1.813664000	2.796210000	-1.153668000
	7	1.729319000	2.003388000	0.524063000
	1	1.392693000	2.881444000	0.891712000
	1	2.717416000	1.800164000	0.550831000
	35	2.982427000	-0.759999000	-0.167175000
	7	-2.165980000	-1.902744000	-0.494403000
	8	-1.834830000	-3.026183000	-0.792721000
	8	-3.274459000	-1.431090000	-0.616559000
	8	-0.744852000	2.525775000	1.160532000
	1	-1.587774000	2.961064000	0.967123000
	8	-1.333401000	-0.013527000	2.050786000
	8	-1.442365000	-1.420493000	1.935295000
TS40	6	-0.892118000	1.222098000	0.181465000
	6	0.597981000	1.017943000	0.051229000
	6	-1.807254000	0.008747000	0.182436000
	1	-2.747055000	0.162112000	-0.345933000
	6	1.065430000	-0.282262000	0.019154000
	6	-1.153975000	-1.275729000	-0.137298000
	6	0.175100000	-1.405740000	-0.205897000
	1	0.608756000	-2.377534000	-0.411229000
	7	-1.304383000	2.320434000	-0.789634000
	8	-1.171312000	3.453637000	-0.395999000
	8	-1.676312000	1.959204000	-1.875295000
	7	1.362862000	2.113872000	0.070968000
	1	0.962306000	3.019611000	0.272758000
	1	2.366875000	2.009876000	0.118471000
	35	2.899491000	-0.563650000	-0.333850000
	7	-2.020014000	-2.429428000	-0.348013000
	8	-1.507495000	-3.487746000	-0.633316000
	8	-3.212221000	-2.234261000	-0.214675000
	8	1.201449000	-0.536761000	2.087288000
	1	0.282538000	-0.427323000	2.386763000
	8	-1.977944000	0.254498000	1.611904000
	8	-1.298144000	1.540996000	1.493108000
TS41	6	-0.761877000	-1.328879000	0.007253000
	6	0.739694000	-1.035242000	-0.183258000
	6	-1.586900000	-0.103005000	-0.390978000
	1	-2.631658000	-0.238478000	-0.107149000
	6	1.214676000	0.276011000	-0.062249000

TS42	6	-1.013435000	1.175874000	0.068633000
	6	0.329803000	1.353239000	0.168078000
	1	0.721294000	2.338680000	0.392951000
	7	-0.952807000	-1.467888000	1.586968000
	8	0.020813000	-1.304824000	2.290255000
	8	-2.065403000	-1.729241000	1.950995000
	7	1.459617000	-2.095084000	-0.437510000
	1	0.945597000	-2.962648000	-0.580652000
	1	2.462531000	-2.052093000	-0.557861000
	35	3.060351000	0.597258000	-0.141600000
	7	-1.904651000	2.322348000	0.226356000
	8	-1.405791000	3.377794000	0.555760000
	8	-3.083663000	2.130749000	0.024284000
	8	-1.139744000	-2.426219000	-0.614391000
	1	-1.808258000	-1.941410000	-1.628822000
	8	-1.486148000	-0.073967000	-1.837067000
	8	-2.158650000	-1.148258000	-2.349589000
	6	-0.075575000	1.428411000	-0.032596000
	6	-1.415575000	0.880882000	-0.479660000
	6	1.044502000	0.383795000	0.117226000
	1	1.792044000	0.804710000	0.793082000
	6	-1.721665000	-0.411935000	-0.168788000
	6	0.513368000	-0.909225000	0.608640000
	6	-0.771630000	-1.283002000	0.441937000
	1	-1.076914000	-2.276845000	0.749722000
	7	-0.279495000	1.990596000	1.440529000
	8	-1.284582000	1.707394000	2.037494000
	8	0.632480000	2.669267000	1.839228000
	7	-2.216791000	1.762792000	-1.083935000
	1	-1.838314000	2.650676000	-1.377271000
	1	-3.127040000	1.478098000	-1.411816000
	35	-3.447203000	-1.076253000	-0.557967000
	7	1.500486000	-1.836817000	1.093047000
	8	1.150980000	-2.910143000	1.525093000
	8	2.673599000	-1.469181000	1.026279000
	8	0.284592000	2.486996000	-0.815985000
	1	1.247024000	2.543742000	-0.901719000
	8	1.661267000	0.205307000	-1.151446000
	8	2.905260000	0.801141000	-1.134552000
	1	3.688250000	-0.343485000	-0.357357000
	8	4.246531000	-0.754258000	-1.113186000
	8	5.417009000	-0.378722000	-1.092156000
TS43				

TS44	
TS45	

Table S3: The electron density ($\rho(r)$ a.u) and Laplacian of electron density ($\nabla^2\rho(r)$ a.u) of reactant complex (RC) transition state and intermediate complex (IC) calculated through AIM analysis at M06-2X/6-311++G(d, p) level of theory.

Reactive Species	Bond type with numbering of atoms	$\rho(r)$ a.u	$(\nabla^2\rho)$ a.u
RC7	N2-H2...O5	0.0170	0.0748
TS7	N2-H2...O5	0.1281	0.0711
IC1	N2-H2...O5	0.0197	0.0719
RC8	H3...O5-H5	0.0170	0.0362
TS8	H3...O5-H5	0.1795	0.0640
IC2	H3...O3-H5	0.0158	0.0532
RC8	H4...O5-H5	0.0136	0.0595
TS9	H4...O5-H5	0.0206	0.0845
IC3	H4...O5-H5	0.0158	0.0532

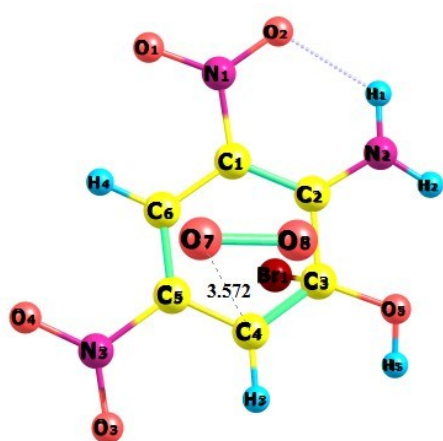
Table S4: The rate constant for the initial reactions calculated using CVT, TST and TST(SCT) methods.

Temp (K)	I1 cm ³ molecule ⁻¹ s ⁻¹			I2 cm ³ molecule ⁻¹ s ⁻¹		
	CVT	TST	TST (SCT)	CVT	TST	TST (SCT)
278	0.15x10 ⁻¹⁸	0.15x10 ⁻¹⁸	0.37x10 ⁻¹⁸	0.13x10 ⁻¹⁶	0.13x10 ⁻¹⁶	0.23x10 ⁻¹⁴
298	0.48x10 ⁻¹⁸	0.49x10 ⁻¹⁸	1.04x10 ⁻¹⁸	0.27x10 ⁻¹⁶	0.27x10 ⁻¹⁶	0.43x10 ⁻¹⁴
318	1.33x10 ⁻¹⁸	1.34x10 ⁻¹⁸	2.55x10 ⁻¹⁸	0.53x10 ⁻¹⁶	0.53x10 ⁻¹⁶	0.79x10 ⁻¹⁴
338	3.27x10 ⁻¹⁸	3.27x10 ⁻¹⁸	5.66x10 ⁻¹⁸	0.94x10 ⁻¹⁶	0.93x10 ⁻¹⁶	1.31x10 ⁻¹⁴
350	7.22x10 ⁻¹⁸	7.21x10 ⁻¹⁸	1.16x10 ⁻¹⁷	1.29x10 ⁻¹⁶	1.28x10 ⁻¹⁶	1.74x10 ⁻¹⁴
400	2.94x10 ⁻¹⁷	2.95x10 ⁻¹⁷	4.20x10 ⁻¹⁷	3.82x10 ⁻¹⁶	3.77x10 ⁻¹⁶	4.75x10 ⁻¹⁴
500	3.20x10 ⁻¹⁷	3.21x10 ⁻¹⁷	7.18x10 ⁻¹⁶	1.71x10 ⁻¹⁵	1.69x10 ⁻¹⁵	5.23x10 ⁻¹⁴
600	1.56x10 ⁻¹⁶	1.57x10 ⁻¹⁶	1.76x10 ⁻¹⁶	4.63x10 ⁻¹⁵	4.55x10 ⁻¹⁵	5.75x10 ⁻¹⁴
700	4.85x10 ⁻¹⁶	4.85x10 ⁻¹⁶	5.21x10 ⁻¹⁶	9.33x10 ⁻¹⁵	9.18x10 ⁻¹⁵	7.19x10 ⁻¹⁴
800	1.13x10 ⁻¹⁵	1.13x10 ⁻¹⁵	1.18x10 ⁻¹⁵	1.58x10 ⁻¹⁴	1.55x10 ⁻¹⁴	7.94x10 ⁻¹⁴
900	2.19x10 ⁻¹⁵	2.18x10 ⁻¹⁵	2.25x10 ⁻¹⁵	2.36x10 ⁻¹⁴	2.32x10 ⁻¹⁴	9.95x10 ⁻¹⁴
1000	3.70x10 ⁻¹⁵	3.70x10 ⁻¹⁵	3.75x10 ⁻¹⁵	3.27x10 ⁻¹⁴	3.20x10 ⁻¹⁴	1.12x10 ⁻¹³

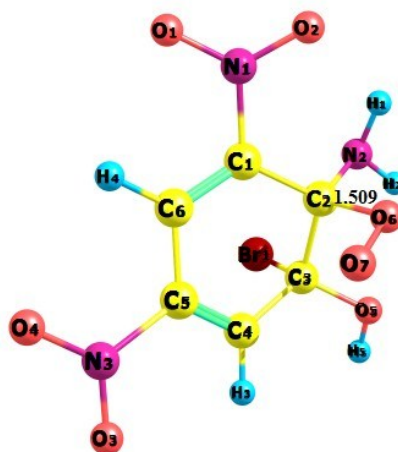
Temp (K)	I3 cm ³ molecule ⁻¹ s ⁻¹			I4 cm ³ molecule ⁻¹ s ⁻¹		
	CVT	TST	TST (SCT)	CVT	TST	TST (SCT)
278	0.09x10 ⁻¹⁶	0.09x10 ⁻¹⁶	0.13x10 ⁻¹⁶	0.18x10 ⁻¹⁶	0.18x10 ⁻¹⁶	0.19x10 ⁻¹⁴
298	0.24x10 ⁻¹⁶	0.23x10 ⁻¹⁶	0.31x10 ⁻¹⁶	0.39x10 ⁻¹⁶	0.38x10 ⁻¹⁶	0.40x10 ⁻¹⁴
318	0.54x10 ⁻¹⁶	0.53x10 ⁻¹⁶	0.68x10 ⁻¹⁶	0.73x10 ⁻¹⁶	0.71x10 ⁻¹⁶	0.72x10 ⁻¹⁴
338	1.11x10 ⁻¹⁶	1.09x10 ⁻¹⁶	1.35x10 ⁻¹⁶	0.95x10 ⁻¹⁶	0.94x10 ⁻¹⁶	0.95x10 ⁻¹⁴
350	2.08x10 ⁻¹⁶	2.04x10 ⁻¹⁶	2.46x10 ⁻¹⁶	1.29x10 ⁻¹⁶	1.26x10 ⁻¹⁶	1.24x10 ⁻¹⁴
400	6.33x10 ⁻¹⁶	6.26x10 ⁻¹⁶	7.15x10 ⁻¹⁶	3.50x10 ⁻¹⁶	3.42x10 ⁻¹⁶	3.41x10 ⁻¹⁴
500	8.15x10 ⁻¹⁶	8.12x10 ⁻¹⁶	8.41x10 ⁻¹⁶	1.89x10 ⁻¹⁵	1.86x10 ⁻¹⁵	5.09x10 ⁻¹⁴
600	1.43x10 ⁻¹⁵	1.43x10 ⁻¹⁵	1.48x10 ⁻¹⁵	5.81x10 ⁻¹⁵	5.71x10 ⁻¹⁵	5.87x10 ⁻¹⁴
700	3.45x10 ⁻¹⁵	3.44x10 ⁻¹⁵	3.51x10 ⁻¹⁵	1.29x10 ⁻¹⁴	1.27x10 ⁻¹⁴	6.81x10 ⁻¹⁴
800	6.66x10 ⁻¹⁵	6.64x10 ⁻¹⁵	6.70x10 ⁻¹⁵	2.34x10 ⁻¹⁴	2.31x10 ⁻¹⁴	7.38x10 ⁻¹⁴
900	1.11x10 ⁻¹⁴	1.10x10 ⁻¹⁴	1.11x10 ⁻¹⁴	3.74x10 ⁻¹⁴	3.67x10 ⁻¹⁴	9.62x10 ⁻¹⁴
1000	1.66x10 ⁻¹⁴	1.66x10 ⁻¹⁴	1.65x10 ⁻¹⁴	5.40x10 ⁻¹⁴	5.31x10 ⁻¹⁴	1.02x10 ⁻¹³

Temp (K)	I5 cm ³ molecule ⁻¹ s ⁻¹			I6 cm ³ molecule ⁻¹ s ⁻¹		
	CVT	TST	TST (SCT)	CVT	TST	TST (SCT)
278	0.14x10 ⁻¹⁶	0.13x10 ⁻¹⁶	0.12x10 ⁻¹⁵	8.12x10 ⁻¹⁴	8.13x10 ⁻¹⁴	7.95x10 ⁻¹³
298	0.20x10 ⁻¹⁶	0.21x10 ⁻¹⁶	0.24x10 ⁻¹⁵	4.40x10 ⁻¹⁴	4.42x10 ⁻¹⁴	7.61x10 ⁻¹³
318	0.38x10 ⁻¹⁶	0.37x10 ⁻¹⁶	0.44x10 ⁻¹⁵	3.08x10 ⁻¹⁴	3.10x10 ⁻¹⁴	7.49x10 ⁻¹³
338	0.66x10 ⁻¹⁶	0.68x10 ⁻¹⁶	0.75x10 ⁻¹⁵	2.69x10 ⁻¹⁴	2.69x10 ⁻¹⁴	6.81x10 ⁻¹³
350	0.99x10 ⁻¹⁶	0.96x10 ⁻¹⁶	1.21x10 ⁻¹⁵	2.49x10 ⁻¹⁴	2.48x10 ⁻¹⁴	5.18x10 ⁻¹³
400	1.77x10 ⁻¹⁶	1.69x10 ⁻¹⁶	2.84x10 ⁻¹⁵	2.36x10 ⁻¹⁴	2.36x10 ⁻¹⁴	4.66x10 ⁻¹³
500	9.30x10 ⁻¹⁶	9.32x10 ⁻¹⁶	6.73x10 ⁻¹⁵	1.99x10 ⁻¹⁴	1.97x10 ⁻¹⁴	2.79x10 ⁻¹³
600	1.71x10 ⁻¹⁵	1.69x10 ⁻¹⁵	1.25x10 ⁻¹⁴	1.74x10 ⁻¹⁴	1.74x10 ⁻¹⁴	2.64x10 ⁻¹³
700	3.22x10 ⁻¹⁵	3.27x10 ⁻¹⁵	3.41x10 ⁻¹⁴	1.62x10 ⁻¹⁴	1.65x10 ⁻¹⁴	2.45x10 ⁻¹³
800	5.07x10 ⁻¹⁵	5.10x10 ⁻¹⁵	7.03x10 ⁻¹⁴	1.47x10 ⁻¹⁴	1.48x10 ⁻¹⁴	2.16x10 ⁻¹³
900	7.12x10 ⁻¹⁵	7.14x10 ⁻¹⁵	7.24x10 ⁻¹⁴	1.22x10 ⁻¹⁴	1.20x10 ⁻¹⁴	1.73x10 ⁻¹³
1000	8.31x10 ⁻¹⁵	8.32x10 ⁻¹⁵	8.64x10 ⁻¹⁴	1.12x10 ⁻¹⁴	1.12x10 ⁻¹⁴	1.38x10 ⁻¹³

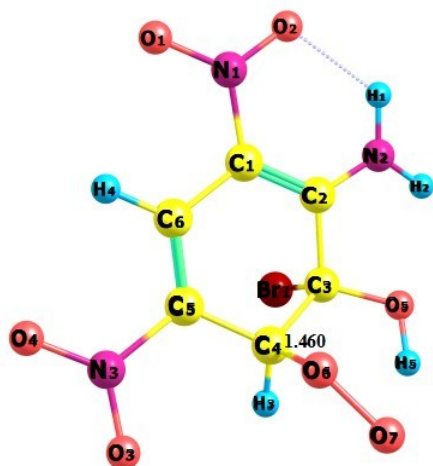
Fig. S2: The optimized structures of the intermediates are involved in the subsequent reaction of I2.



I2 + O₂



I11

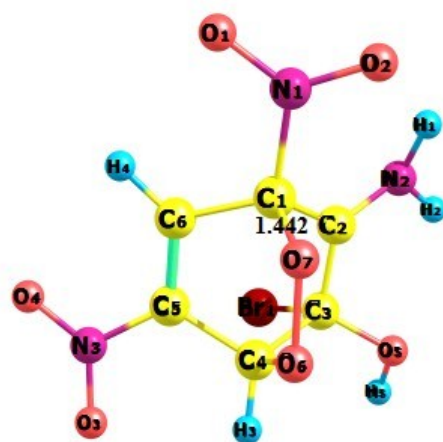


I12

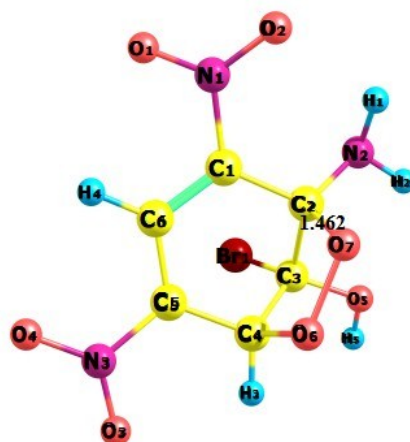


I13

Fig. S3: The optimized structure of the intermediates and products involved in the subsequent reaction of I12.



I14



I15

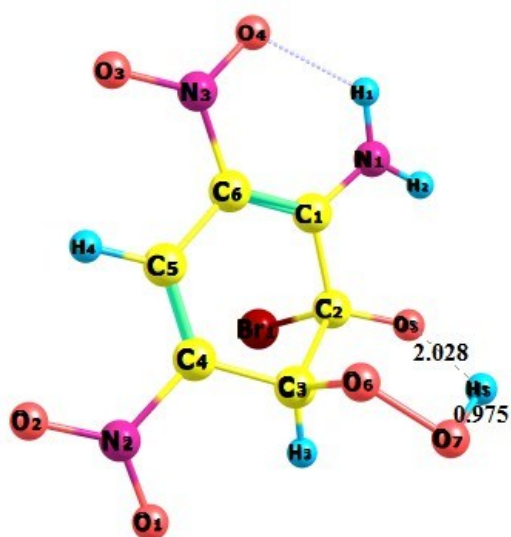
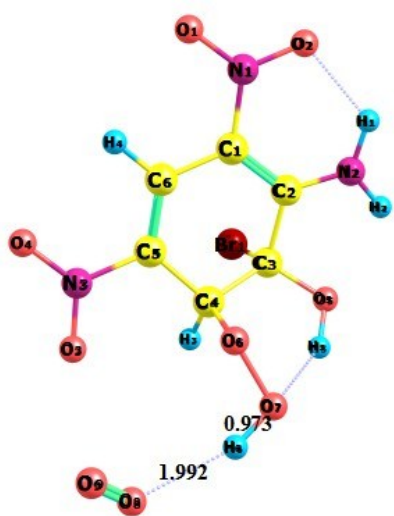
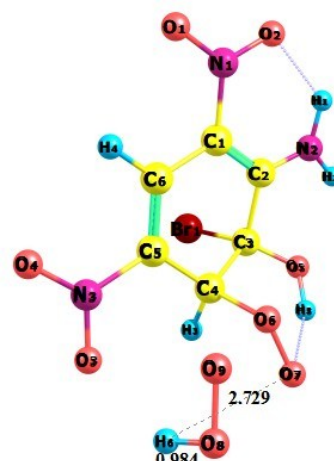
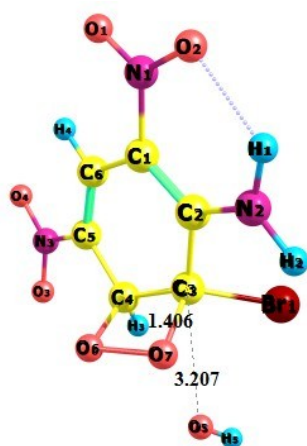
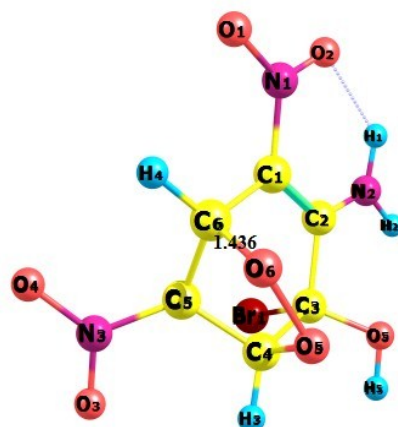
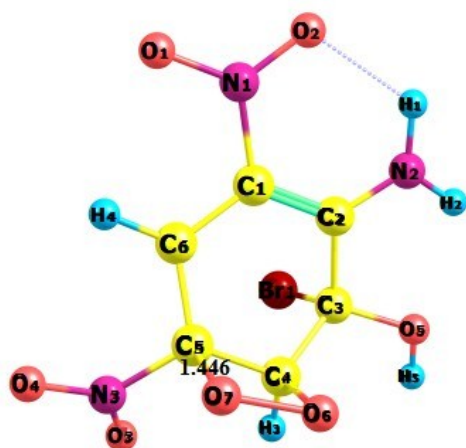


Fig. S4: The optimized structures of the intermediates are involved in the subsequent reaction of I4.

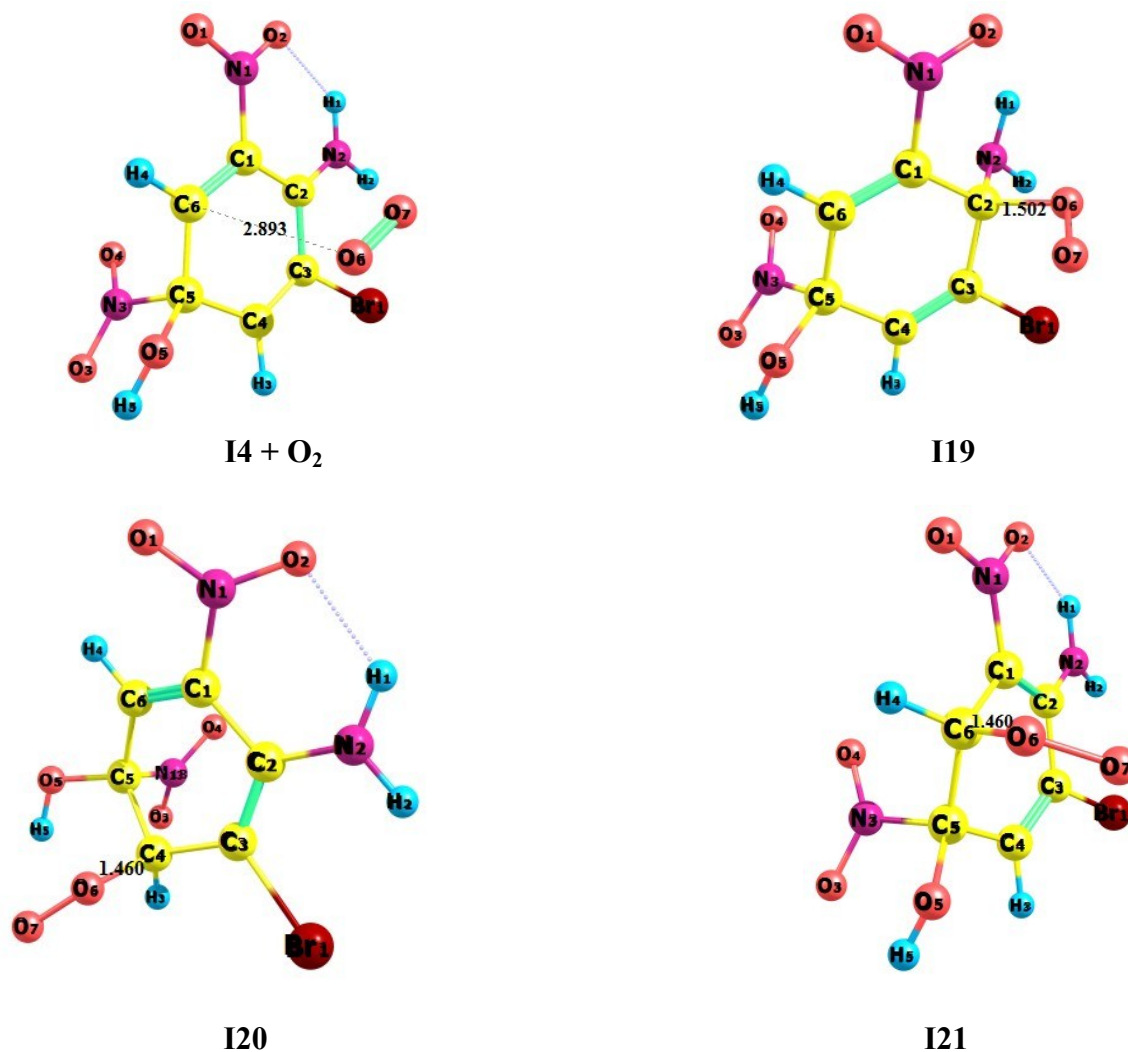
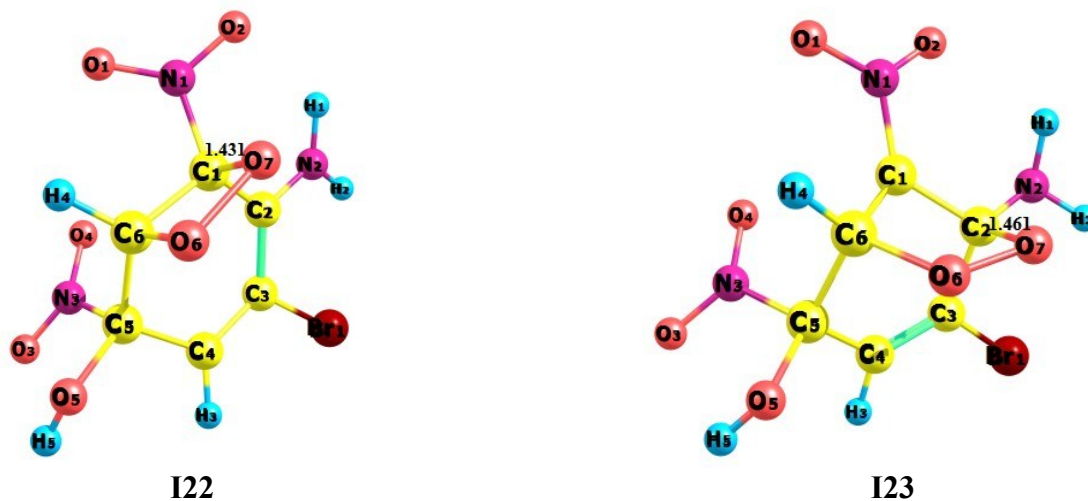
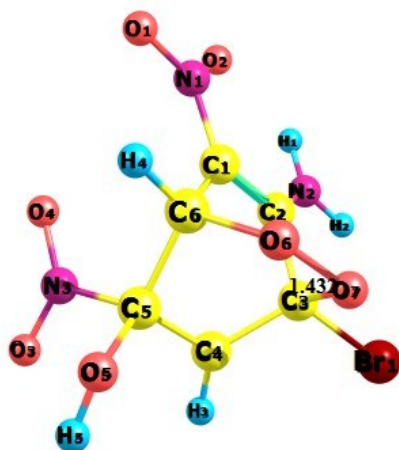
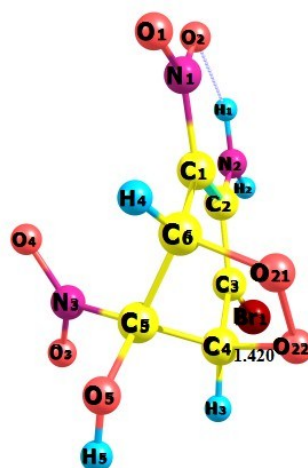


Fig. S5: The optimized structure of the intermediates and products involved in the subsequent reaction of I21.

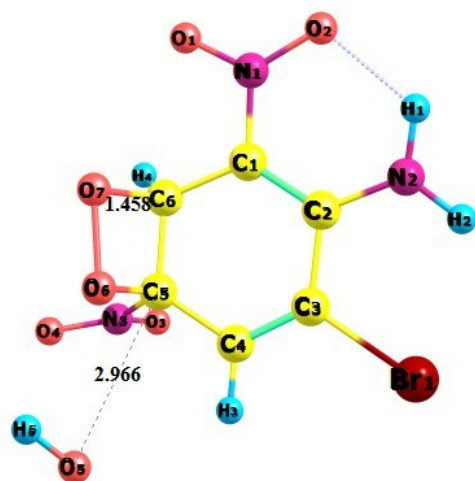




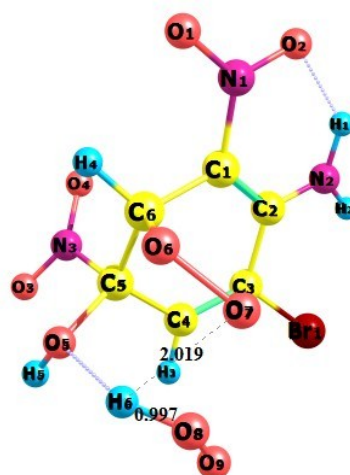
I24



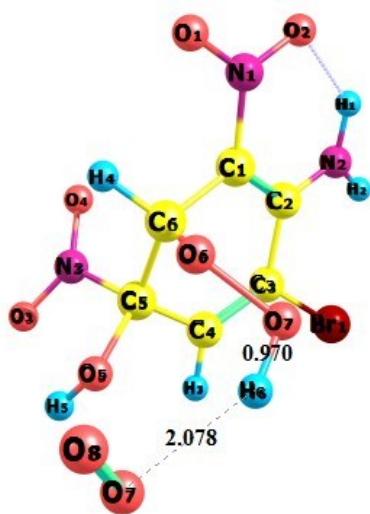
I25



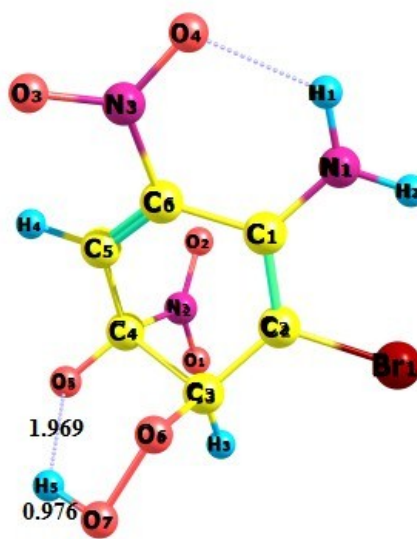
P3 + OH



I21 + HO₂

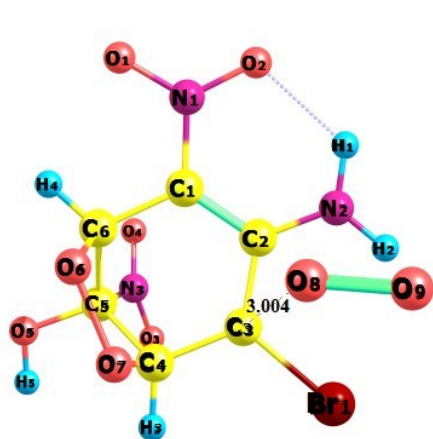


P4 + O₂

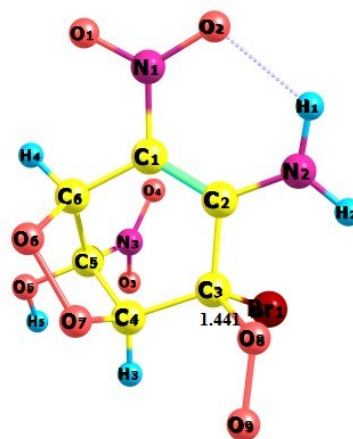


I26

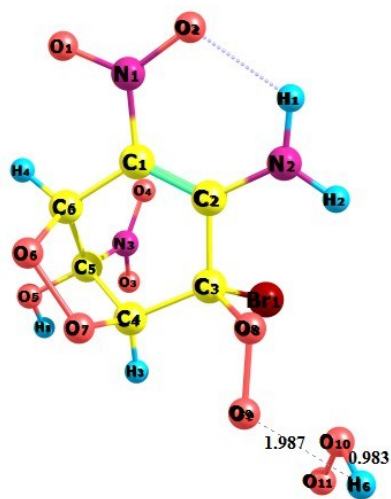
Fig. S6: The optimized structure of the intermediates and products involved in the subsequent reaction of I25.



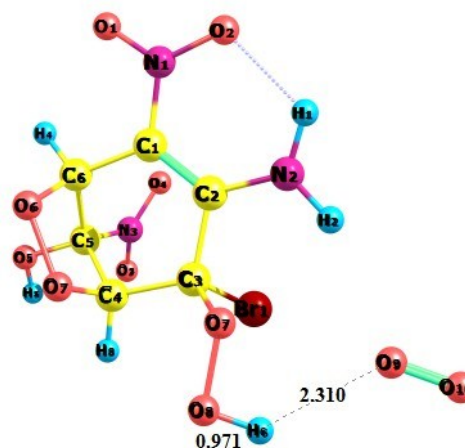
I25 + O₂



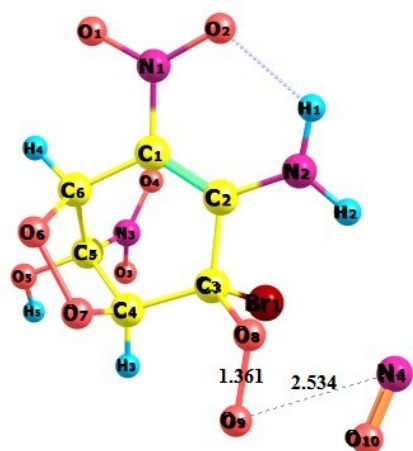
I27



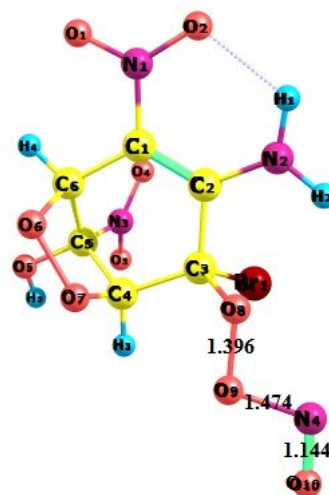
I27 + HO₂



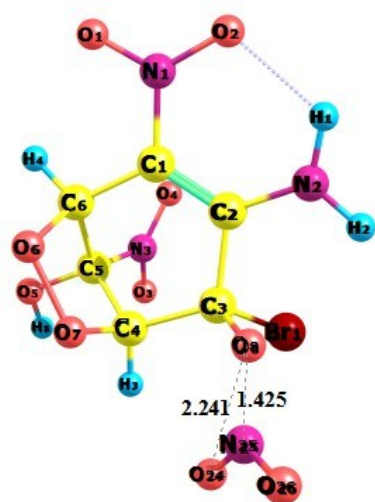
P5



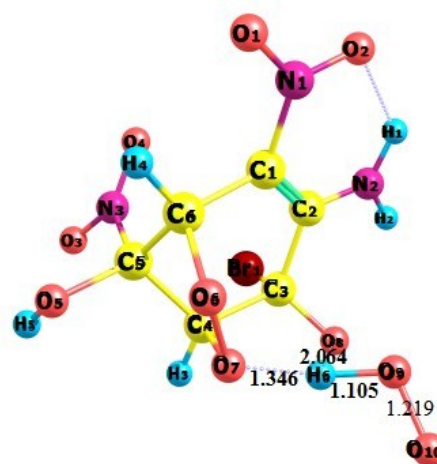
I27 + NO



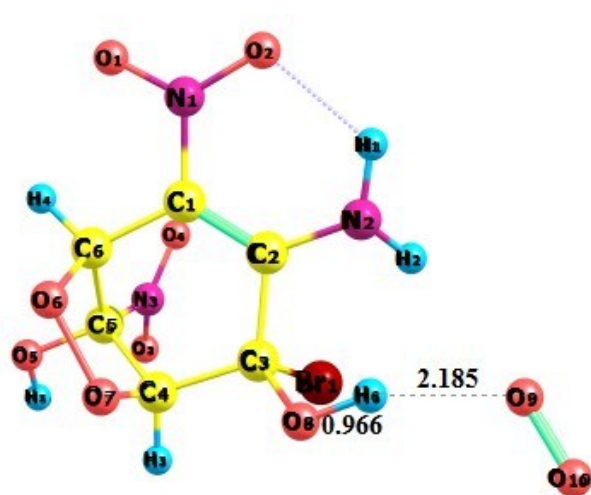
I28



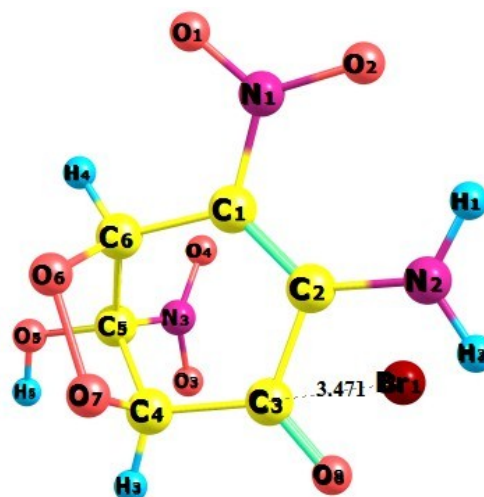
I29 + NO₂



I29 + HO₂

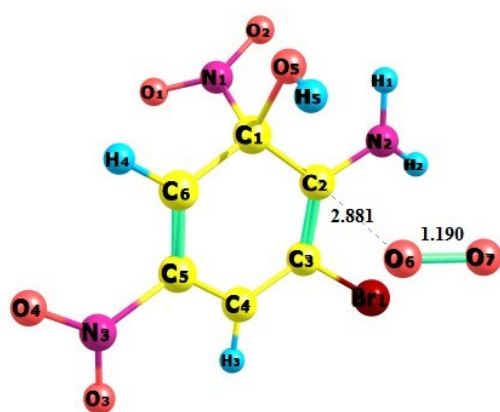


P6 + O₂

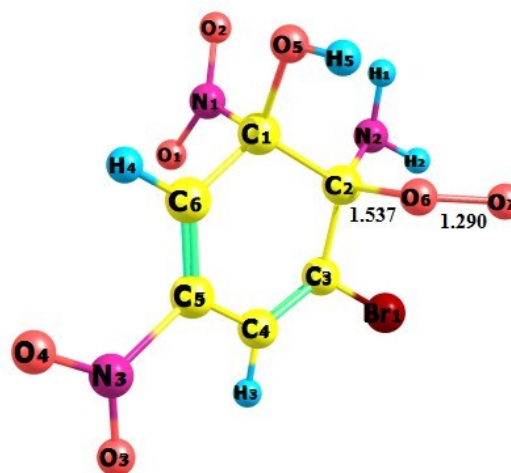


P7 + Br

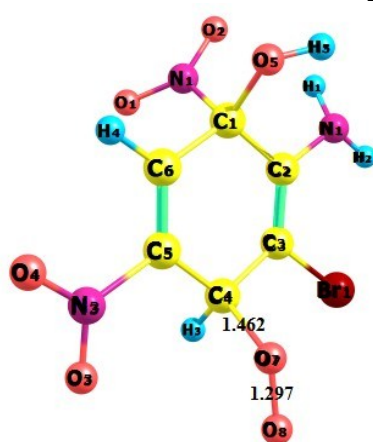
Fig. S7: The optimized structures of the intermediates are involved in the subsequent reaction of I6.



I6 + O₂



I30

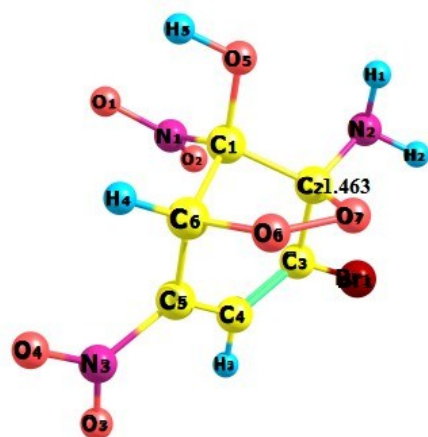


I31

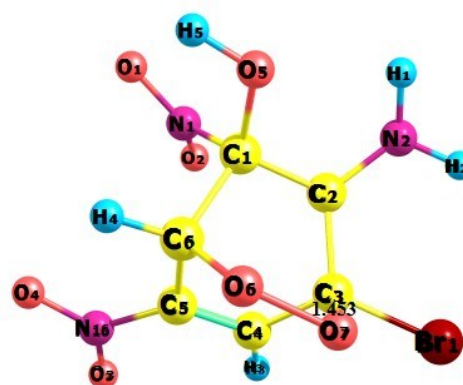


I32

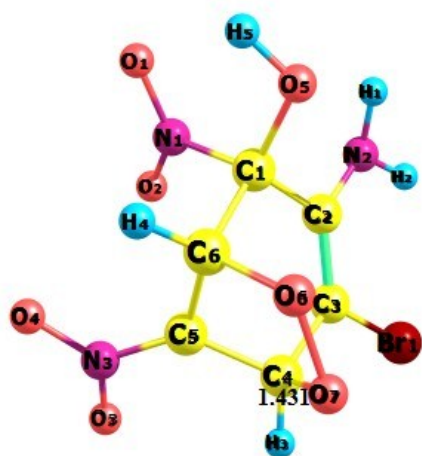
Fig. S8: The optimized structure of the intermediates and products involved in the subsequent reaction of I32.



I34



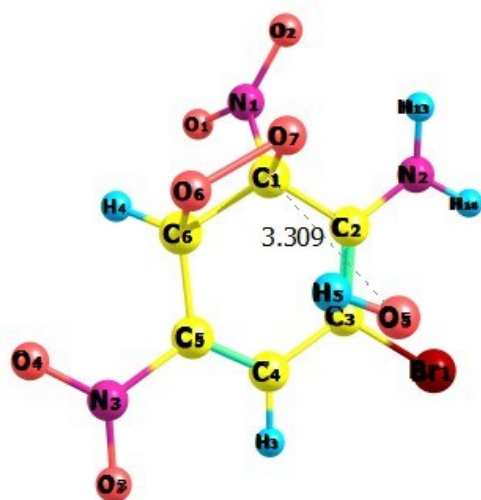
I35



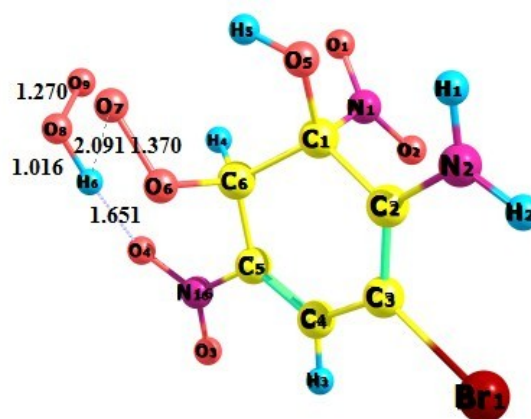
I36



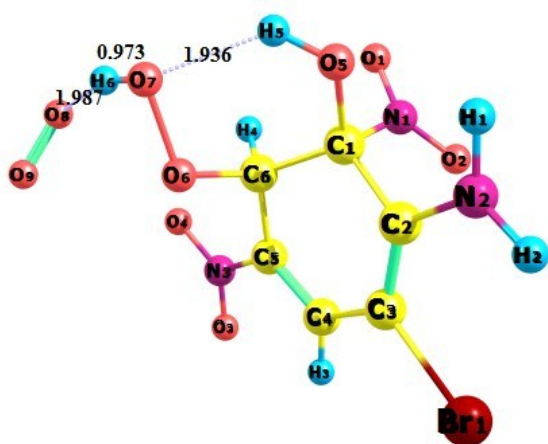
I37



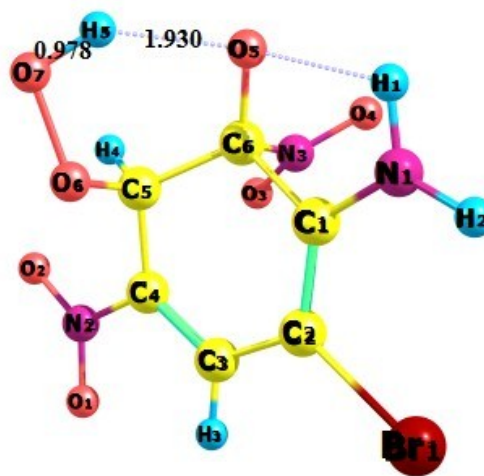
P8 + OH



I32 + HO₂



P9 + O₂



I38