Electronic Supplementary Information (ESI)

Catalytic Effect of Water and Formic Acid on the Reaction of Carbonyl Sulfide with Dimethyl Amine Under Tropospheric Conditions

Parandaman Arathala, and Rabi A. Musah*

University at Albany—State University of New York, Department of Chemistry, 1400 Washington Avenue, Albany, NY 12222, USA

This section contains: Tables S1-S11 presents the optimized geometries of all the stationary points, calculated total electronic energies including zero-point energy corrections, vibrational frequencies and rotational constants, and imaginary frequencies of various TSs as discussed in the text at M06-2X level, relative energies of complexes at various levels, temperature dependent unimolecular and effective rate coefficients using CVT/SCT method, equilibrium constants. Figure S1-S2 presents the optimized geometries for the reaction of OCS + NH_3 and OCS + MA, Figure S3-S8 presents the IRC plots for the OCS + DMA, OCS + DMA + H_2O, and OCS + DMA + FA reactions.

Table S1: Calculated total electronic energies for reactants, their complexes, transition states (TSs), product complexes, and products at the M06-2X, and CCSD(T) levels. Zero-point energy (ZPE) corrections are given at the M06-2X level.

Species	M06-2X/aug-cc-pVTZ	ZPE (M06-2X)	CCSD(T)/aug-cc-pVTZ
OCS	-511.542731	0.009389	-510.929754
NH_3	-56.5529640	0.034438	-56.480529
OCS••NH_3 (RC1)	-568.098717	0.044869	-567.413331
OCS••NH_3 (TS1)	-568.036383	0.042968	-567.348377
$NH_2C(O)SH$ (P1)	-568.098674	0.045321	-567.409091
CH_3-NH_2 (MA)	-95.845531	0.064401	-95.706066
OCS••MA (RC2)	-607.392730	0.074849	-606.640221
OCS••MA (TS2)	-607.339363	0.071868	-606.586236
$(CH_3)NHC(O)SH$ (P2)	-607.399453	0.074060	-606.643886
$(CH_3)_2$-NH (DMA)	-135.144195	0.093048	-134.938202
OCS••DMA (RC3)	-646.692474	0.103418	-645.873542
OCS••DMA (TS3)	-646.644828	0.100066	-645.826953
$(CH_3)_2NHC(O)SH$ (P3)	-646.699069	0.102865	-645.878132
OCS••NH_3 (TS4)	-568.025405	0.044633	-567.336344
$NH_2C(S)OH$ (P4)	-568.099281	0.049615	-567.407255
OCS••MA (TS5)	-607.329466	0.073503	-606.575059
$(CH_3)NHC(S)OH$ (P5)	-607.401392	0.078153	-606.643350
OCS••DMA (TS6)	-646.635504	0.101612	-645.816160
$(CH_3)_2NHC(S)OH$ (P6)	-646.700094	0.106433	-645.877014
H_2O	-76.4301050	0.021547	-76.342290
Formic acid (FA)	-189.769567	0.034264	-189.517431
OCS••NH_3••H_2O (PRC1)	-644.518946	0.073267	-643.742406
OCS••NH_3••H_2O (TS7)	-644.499981	0.068889	-643.720488
OCS••NH_3••H_2O (PC1)	-644.537254	0.069640	-643.760383
OCS••NH_3••H_2O (PRC2)	-644.539467	0.070059	-643.766483
OCS••NH_3••H_2O (TS8)	-644.498181	0.069480	-643.717947
OCS••NH_3••H_2O (PC2)	-644.531978	0.073626	-643.752398
OCS••NH_3••FA (PRC3)	-757.865587	0.084999	-756.926060

OCS••NH_3••FA (TS9)	-757.854667	0.077947	-756.911905
OCS••NH_3••FA (PC3)	-757.880590	0.082815	-756.940053
OCS••NH_3••FA (PRC4)	-757.866406	0.085454	-756.926661
OCS••NH_3••FA (TS10)	-757.858635	0.079789	-756.915107
OCS••NH_3••FA (PC4)	-757.875054	0.086329	-756.932800
OCS••MA••H_2O (PRC5)	-683.822613	0.102729	-682.980827
OCS•• MA••H_2O (TS11)	-683.799972	0.097000	-682.955333
OCS•• MA••H_2O (PC5)	-683.840503	0.098585	-682.997175
OCS••MA••H_2O (PRC6)	-683.822704	0.103452	-682.980668
OCS••MA••H_2O (TS12)	-683.798742	0.097875	-682.953674
OCS••MA••H_2O (PC6)	-683.826777	0.102397	-682.981308
OCS•• MA••FA (PRC7)	-797.169553	0.114294	-796.164720
OCS••MA••FA (TS13)	-797.156284	0.106321	-796.149897
OCS••MA••FA (PC7)	-797.184385	0.110650	-796.177961
OCS••MA••FA (PRC8)	-797.171337	0.114729	-796.166385
OCS••MA••FA (TS14)	-797.162791	0.109252	-796.154712
OCS••MA••FA (PC8)	-797.187831	0.114524	-796.179650
OCS••H_2O (RC4)	-587.975893	0.032228	-587.274924
OCS••H_2O (RC5)	-587.976208	0.032337	-587.275340
OCS••DMA••H_2O (PRC9)	-723.127845	0.131274	-722.221333
OCS••DMA••H_2O (TS15)	-723.101283	0.124315	-722.192613
OCS••DMA••H_2O (PC9)	-723.136237	0.126528	-722.227886
OCS••DMA••H_2O (PRC10)	-723.125989	0.131440	-722.219281
OCS••DMA••H_2O (TS16)	-723.101919	0.125765	-722.192500
OCS••DMA••H_2O (PC10)	-723.141615	0.130608	-722.230850
OCS••FA (RC7)	-700.452502	0.044553	-701.317168
OCS••FA (RC8)	-700.453771	0.044746	-701.318614
OCS••DMA••FA (PRC11)	-836.475479	0.142588	-835.406178
OCS••DMA••FA (TS17)	-836.460273	0.134794	-835.390218
OCS••DMA••FA (PC11)	-836.478002	0.138462	-835.407187
OCS••DMA••FA (PRC12)	-836.475257	0.142800	-835.405986
OCS••DMA••FA (TS18)	-836.465054	0.137686	-835.392515

OCS••DMA••FA (PC12)	-836.487044	0.142245	-835.401016

Table S2: Imaginary frequencies of all transition states obtained at the M06-2X/aug-cc-pVTZ level of theory.

Transition State	M06-2X/aug-cc-pVTZ
OCS••NH_3 (TS1)	1500
OCS••MA (TS2)	1473
OCS••DMA (TS3)	1437
OCS••NH_3 (TS4)	1689
OCS••MA (TS5)	1711
OCS••DMA (TS6)	1724
OCS••NH_3••H_2O (TS7)	1017
OCS••NH_3••FA (TS8)	1200
OCS••NH_3••H_2O (TS9)	1394
OCS••NH_3••FA (TS10)	1099
OCS••MA••H_2O (TS11)	1165
OCS••MA••H_2O (TS12)	1494
OCS••MA••FA (TS13)	1127
OCS••MA••FA (TS14)	714
OCS••DMA••H_2O (TS15)	1361
OCS••DMA••H_2O (TS16)	1463
OCS••DMA••FA (TS17)	812
OCS••DMA••FA (TS18)	565

Table S3: Calculated rotational constants (GHz) for reactants, their complexes, transition states (TS), and products at the M06-2X/aug-cc-pVTZ level of theory.

Species	A	B	C
OCS	6.11		
NH_3	299.81	299.63	188.88
OCS••NH_3 (RC1)	7.53	3.07	2.21
OCS••NH_3 (TS1)	10.17	5.31	3.56
$NH_2C(O)SH$ (P1)	11.09	5.07	3.48
CH_3-NH_2 (MA)	104.28	22.87	21.97
OCS••MA (RC2)	5.38	2.08	1.69
OCS••MA (TS2)	12.43	4.66	3.45
$(CH_3)NHC(O)SH$ (P2)	11.25	5.17	3.54
$(CH_3)_2$-NH (DMA)	34.59	9.44	8.31
OCS••DMA (RC3)	4.43	1.92	1.83
OCS••DMA (TS3)	4.20	2.11	1.96
$(CH_3)_2NHC(O)SH$ (P3)	4.49	2.37	1.58
OCS••NH_3 (TS4)	12.43	4.66	3.45
$NH_2C(S)OH$ (P4)	11.25	5.17	3.54
OCS••MA (TS5)	5.79	3.30	2.27
$(CH_3)NHC(S)OH$ (P5)	5.39	3.73	2.23
OCS••DMA (RC4)	3.59	1.65	1.29
OCS••DMA (TS6)	3.89	2.25	1.99
$(CH_3)_2NHC(S)OH$ (P6)	4.44	2.43	1.60
H_2O	833.84	430.93	284.10
Formic acid (FA)	78.05	12.21	10.56
OCS••NH_3••H_2O (PRC1)	4.28	2.54	1.79
OCS••NH_3••H_2O (TS7)	4.72	3.07	2.01
OCS••NH_3••H_2O (PC1)	5.09	2.05	1.47
OCS••NH_3••H_2O (PRC2)	4.60	1.59	1.19
OCS••NH_3••H_2O (TS8)	9.89	2.03	1.74
OCS••NH_3••H_2O (PC2)	10.94	1.59	1.40
OCS••NH_3••FA (PRC3)	3.11	1.23	0.96
OCS••NH_3••FA (TS9)	3.31	1.42	1.07
OCS••NH_3••FA (PC3)	3.33	1.15	0.98
OCS••NH_3••FA (PRC4)	5.01	0.94	0.82
OCS••NH_3••FA (TS10)	5.03	1.07	0.94
OCS••NH_3••FA (PC4)	4.80	0.98	0.89
OCS••MA••H_2O (PRC5)	2.57	2.19	1.33
OCS•• MA••H_2O (TS11)	3.13	2.33	1.44
OCS•• MA••H_2O (PC5)	2.70	2.10	1.20
OCS••MA••H_2O (PRC6)	4.20	1.59	1.30
OCS••MA••H_2O (TS12)	4.15	1.88	1.42

OCS••MA••H_2O (PC6)	3.89	1.61	1.15
OCS•• MA••FA (PRC7)	2.25	1.05	0.81
OCS••MA••FA (TS13)	2.28	1.22	0.99
OCS••MA••FA (PC7)	2.12	1.00	0.73
OCS••MA••FA (PRC8)	2.85	0.88	0.76
OCS••MA••FA (TS14)	3.00	0.96	0.88
OCS••MA••FA (PC8)	2.92	0.81	0.64
OCS••DMA••H_2O (PRC9)	1.99	1.84	1.17
OCS••DMA••H_2O (TS15)	2.32	1.88	1.32
OCS••DMA••H_2O (PC9)	2.40	1.34	1.16
OCS••DMA••H_2O (PRC10)	2.63	1.43	1.12
OCS••DMA••H_2O (TS16)	2.68	1.65	1.28
OCS••DMA••H_2O (PC10)	2.10	1.66	1.44
OCS••DMA••FA (PRC11)	1.70	0.93	0.69
OCS••DMA••FA (TS17)	1.67	1.13	0.82
OCS••DMA••FA (PC11)	1.54	0.92	0.78
OCS••DMA••FA (PRC12)	2.07	0.79	0.65
OCS••DMA••FA (TS18)	2.14	0.91	0.76
OCS••DMA••FA (PC12)	1.47	1.07	0.84

Table S4: Calculated positive frequencies (cm^{-1}) for reactants, their complexes, transition states (TSs) and products at the M06-2X/aug-cc-pVTZ level of theory.

Species	Frequencies
OCS	540 540 886 2156
NH_3	1033 1659 1660 3505 3629 3630
OCS••NH_3 (RC1)	30 66 81 110 173 524 540 888 1045 1658 1660 2153 3506 3630 3632
OCS••NH_3 (TS1)	-1500 176 457 532 566 695 941 1042 1081 1142 1558 1739 1903 3465 3566
$NH_3C(O)SH$ (P1)	79 245 360 466 511 674 693 906 1108 1295 1615 1821 2749 3616 3756
CH_3-NH_2 (MA)	292 831 973 1085 1174 1344 1459 1508 1525 1659 3024 3103

	3137 3538 3617
OCS••MA (RC2)	41 68 102 120 131 307 520 542 833 883 974 1084 1175 1343 1459 1508 1527 1655 2161 3029 3098 3134 3539 3620
OCS••MA (TS2)	-1473 57 210 257 465 529 595 718 840 996 1066 1125 1155 1183 1375 1451 1498 1514 1727 1897 3074 3148 3170 3497
$NH_3C(S)OH$ (P2)	59 132 182 238 370 384 466 692 830 875 1061 1160 1197 1245 1459 1485 1513 1544 1801 2747 3076 3137 3174 3681
$(CH_3)_2$-NH (DMA)	230 276 392 772 962 1037 1107 1193 1198 1271 1440 1470 1477 1493 1504 1519 1522 2983 2984 3086 3088 3136 3136 3565
OCS••DMA (RC3)	26 186 210 243 249 284 384 465 556 663 842 939 1049 1082 1094 1176 1250 1275 1434 1458 1464 1497 1503 1512 1515 1841 3075 3077 3158 3158 3175 3176 3499
OCS••DMA (TS3)	-1437 62 228 239 243 292 330 485 559 693 703 947 975 1014 1067 1125 1217 1241 1279 1432 1465 1487 1498 1504 1516 1731 1899 3055 3057 3133 3133 3157 3158
$(CH_3)NH_2C(O)SH$ (P3)	79 101 128 212 285 350 392 450 462 676 696 896 976 1096 1126 1136 1173 1313 1420 1443 1477 1501 1506 1509 1538 1777 2750 3048 3052 3109 3122 3160 3194
OCS••NH_3 (TS4)	-1689 311 377 521 619 856 1002 1070 1083 1382 1566 1571 2136 3503 3596

$(CH_3)NH_2C(S)OH$ (P4)	318 405 482 523 619 665 797 1047 1202 1386 1494 1642 3615 3759 3825
OCS••MA (TS5)	-1711 122 216 232 418 607 635 759 925 1045 1121 1150 1188 1343 1426 1455 1499 1511 1552 2132 3077 3157 3174 3519
$(CH_3)_2NHC(O)SH$ (P5)	127 186 246 440 457 550 572 666 752 1060 1162 1178 1241 1282 1440 1482 1499 1516 1601 3074 3137 3172 3639 3828
OCS••DMA (RC4)	30 80 94 108 132 232 284 394 517 540 771 882 962 1039 1107 1195 1197 1271 1440 1470 1474 1492 1504 1517 1523 2157 2991 2993 3076 3086 3134 3135 3567
OCS••DMA (TS6)	-1724 92 224 226 245 278 367 515 620 693 710 995 1065 1080 1095 1180 1221 1298 1378 1436 1469 1487 1495 1506 1511 1544 2133 3061 3064 3142 3143 3164 3166
$(CH_3)_2NHC(S)OH$ (P6)	58 102 140 252 279 412 466 511 580 665 715 960 1093 1127 1133 1172 1242 1305 1381 1451 1455 1484 1504 1506 1514 1619 3061 3074 3115 3138 3167 3215 3821
H_2O	1618 3868 3972
Formic acid (FA)	645 671 1075 1162 1317 1413 1870 3096 3791
OCS••NH_3••H_2O (PRC1)	33 158 168 187 237 281 356 404 524 540 594 775 905 975 1334 1612 1621 1658 1849 3265 3508 3590 3661 3926
OCS••NH_3••H_2O (TS7)	-1017 79 360 390 459 483 494 584 640 697 722 934

	1056 1165 1254 1422 1500 1588 1670 1807 2020 3486 3574 3857
OCS••NH_3••H_2O (PC1)	39 84 114 150 157 169 350 386 394 466 590 678 729 932 1138 1311 1615 1631 1809 2719 3574 3715 3860 3960
OCS••NH_3••H_2O (PRC2)	14 61 84 90 96 169 187 192 224 456 531 538 645 882 1096 1637 1655 1662 2163 3499 3619 3625 3691 3938
OCS••NH_3••H_2O (TS8)	-1394 63 332 362 436 543 593 623 690 741 755 1016 1057 1154 1280 1400 1534 1581 1639 1718 2017 3492 3578 3895
OCS••NH_3••H_2O (PC2)	43 105 129 173 232 284 347 416 525 569 662 747 816 1056 1237 1399 1517 1617 1637 3590 3675 3743 3851 3948
OCS••NH_3••FA (PRC3)	28 53 133 154 187 229 307 372 479 555 569 704 807 876 986 1039 1098 1276 1405 1421 1435 1616 1656 1775 1830 3003 3102 3156 3486 3575
OCS••NH_3••FA (TS9)	-1200 55 89 155 268 354 424 480 531 568 622 708 770 962 1015 1077 1085 1115 1218 1370 1407 1441 1496 1589 1656 1768 1821 3120 3479 3569
OCS••NH_3••FA (PC3)	53 63 98 146 159 175 352 394 466 546 627 687 708 728 853 951 1089 1144 1230 1282 1383 1431 1623 1818 1827 2709 3107 3514 3541 3649
OCS••NH_3••FA (PRC4)	18 57 136 169 204 220 280 400 483 562 597 708 858 967 988 1063 1105 1293 1411 1423 1452 1620 1650 1705 1787 3029 3103 3156 3497 3571

OCS••NH_3••FA (TS10)	-1099 62 76 181 266 352 399 483 585 627 673 760 811 1024 1061 1101 1176 1256 1296 1406 1434 1535 1581 1601 1644 1705 1789 3107 3470 3562
OCS••NH_3••FA (PC4)	56 66 124 153 188 210 420 511 528 637 700 757 784 823 934 1095 1105 1221 1257 1384 1413 1440 1518 1627 1799 3117 3364 3495 3522 3644
OCS••MA••H_2O (PRC5)	33 88 153 173 196 225 259 330 361 489 539 559 586 836 870 1049 1092 1139 1312 1374 1455 1501 1505 1618 1658 1833 3100 3185 3199 3277 3526 3651 3924
OCS•• MA••H_2O (TS11)	-1165 71 174 207 275 382 420 474 498 521 587 700 755 939 996 1096 1149 1183 1230 1351 1405 1442 1482 1498 1516 1639 1807 1985 3089 3166 3176 3510 3860
OCS•• MA••H_2O (PC5)	41 76 88 112 143 151 242 247 307 328 375 461 636 719 826 891 1066 1160 1200 1267 1459 1487 1517 1575 1626 1804 2751 3073 3131 3172 3555 3846 3939
OCS••MA••H_2O (PRC6)	39 77 176 193 204 218 253 381 414 462 567 621 676 822 930 1036 1121 1136 1321 1361 1453 1505 1507 1608 1615 1759 3094 3180 3193 3351 3528 3669 3938
OCS••MA••H_2O (TS12)	-1494 67 144 205 258 350 441 511 603 656 704 736 760 935 1053 1076 1156 1167 1233 1373 1392 1463 1499 1517 1576 1592 1673 1971 3078 3160 3166 3541 3908

OCS••MA••H_2O (PC6)	51 124 142 155 176 197 249 267 444 462 540 575 634 699 753 1076 1159 1176 1240 1281 1446 1485 1512 1533 1609 1637 3072 3133 3173 3510 3815 3819 3947
OCS•• MA••FA (PRC7)	28 36 81 147 159 195 201 224 252 406 505 592 684 710 819 908 948 1033 1100 1143 1153 1285 1352 1400 1425 1442 1451 1503 1511 1641 1775 1803 3032 3093 3106 3153 3184 3190 3500
OCS••MA••FA (TS13)	-1127 63 88 125 167 186 238 255 375 429 474 576 670 721 771 953 983 1035 1046 1075 1097 1183 1277 1317 1398 1400 1432 1472 1506 1512 1546 1679 1776 1820 3075 3091 3175 3191 3496
OCS••MA••FA (PC7)	33 56 71 95 135 139 149 173 245 342 369 454 603 679 702 789 827 881 1061 1088 1157 1198 1223 1272 1372 1429 1459 1488 1515 1577 1815 1830 2744 3073 3106 3137 3177 3539 3566
OCS••MA••FA (PRC8)	38 39 86 138 173 201 215 225 263 408 521 626 696 712 863 957 993 1035 1107 1139 1167 1299 1347 1412 1425 1451 1459 1505 1509 1608 1687 1787 3030 3093 3105 3150 3186 3189 3519
OCS••MA••FA (TS14)	-714 63 90 135 180 196 253 274 345 380 582 675 750 793 804 983 1031 1100 1121 1170 1198 1270 1384 1400 1415 1441 1494 1508 1525 1557 1614 1625 1726 1818 3080 3090 3179 3186 3519

OCS••MA••FA (PC8)	20 54 98 143 147 163 163 204 247 458 525 575 646 691 728 754 829 1078 1089 1160 1167 1226 1234 1288 1398 1437 1447 1486 1511 1540 1635 1825 3072 3108 3134 3175 3457 3555 3800
OCS••DMA••H_2O (PRC9)	18 49 147 172 196 207 242 252 294 310 363 450 547 563 598 687 884 937 1054 1080 1167 1181 1260 1366 1434 1463 1474 1496 1507 1516 1520 1620 1806 3085 3089 3172 3173 3184 3191 3345 3602 3924
OCS••DMA••H_2O (TS15)	-1361 56 123 208 235 252 281 352 400 440 490 511 556 641 707 762 940 1004 1065 1113 1176 1196 1221 1244 1284 1414 1438 1484 1486 1501 1508 1520 1612 1797 1905 3062 3076 3141 3150 3168 3173 3874
OCS••DMA••H_2O (PC9)	37 49 103 127 138 148 168 201 256 285 293 356 393 451 463 680 696 885 969 1093 1130 1134 1179 1301 1403 1444 1479 1499 1503 1511 1534 1608 1778 2744 3051 3053 3126 3137 3165 3193 3825 3946
OCS••DMA••H_2O (PRC10)	34 49 149 181 190 200 244 253 266 336 399 464 522 565 606 684 845 968 1056 1076 1170 1181 1268 1376 1432 1463 1468 1493 1504 1511 1516 1607 1756 3082 3084 3168 3169 3184 3190 3363 3685 3939
OCS••DMA••H_2O (TS16)	-1463 49 125 218 253 264 278 301 420 444 526 612 661 672 721 745 982 1066 1077 1111 1182 1206 1260 1294 1367 1437 1481 1483 1498 1505 1517 1540 1578 1674 1953 3070 3077 3153 3157 3167 3170 3910

OCS••DMA••H_2O (PC10)	47 63 85 108 121 139 161 284 301 330 423 438 469 510 570 674 715 956 1091 1123 1132 1180 1242 1303 1379 1443 1453 1486 1504 1507 1512 1630 1634 3062 3070 3133 3140 3189 3216 3751 3823 3934
OCS••DMA••FA (PRC11)	19 29 59 111 153 182 195 209 249 259 292 310 457 552 646 696 709 898 917 936 1054 1080 1099 1173 1181 1262 1282 1382 1424 1432 1446 1461 1479 1496 1508 1520 1528 1779 1802 3062 3087 3088 3109 3174 3175 3187 3188 3251
OCS••DMA••FA (TS17)	-812 62 80 119 139 181 225 232 260 287 347 368 457 463 612 692 758 779 934 977 1028 1061 1099 1106 1166 1202 1255 1301 1353 1395 1433 1442 1485 1488 1493 1509 1528 1596 1682 1789 1827 3054 3082 3093 3165 3179 3192 3193
OCS••DMA••FA (PC11)	21 31 45 91 119 129 149 172 181 252 286 298 395 451 469 677 688 697 847 888 967 1085 1086 1123 1129 1178 1210 1289 1370 1377 1426 1447 1478 1496 1497 1509 1528 1784 1845 2733 3054 3055 3092 3131 3141 3179 3190 3493
OCS••DMA••FA (PRC12)	12 32 68 102 163 197 202 215 250 259 264 351 515 548 618 697 709 883 976 985 1055 1078 1106 1181 1191 1268 1294 1414 1431 1434 1460 1464 1477 1493 1505 1518 1535 1686 1787 3077 3084 3086 3109 3171 3172 3177 3187 3196
OCS••DMA••FA (TS18)	-565 63 84 128 153 193 250 257 283 292 350 364 431 551 686 732 778 819

	957	1061	1100	1108	1116	1203
	1222	1235	1282	1395	1430	1440
	1455	1484	1489	1500	1506	1519
	1569	1587	1710	1722	1973	3072
	3081	3089	3166	3172	3186	3194
OCS••DMA••FA (PC12)	15	59	74	92	97	129
	146	153	171	295	302	423
	467	507	571	667	683	715
	812	952	1089	1094	1123	1133
	1178	1227	1245	1306	1372	1380
	1426	1445	1454	1486	1502	1508
	1513	1645	1828	3071	3075	3083
	3137	3146	3186	3217	3417	3819

Table S5: The MO6-2X/aug-cc-pVTZ level optimized geometries of reactants, reactant complexes, transition states, product complexes, and products involved in the OCS with three different amine addition reactions catalyzed by a single water and a formic acid molecule.

OCS

C	-0.25245000	-0.18581100	0.00000000
S	1.31213500	-0.18581100	0.00000000
O	-1.40113900	-0.18581100	0.00000000

NH_3

N	-0.46146500	-0.60816500	0.00013400
H	-0.08719100	-1.54889000	-0.00020300
H	-0.08718100	-0.13755800	0.81465800
H	-0.08713600	-0.13783300	-0.81458900

CH_3-NH_2 (MA)

N	-0.44150700	-0.58541500	0.00870800
H	-0.07863200	-1.52725800	0.07436100
H	-0.14610600	-0.10073800	0.84588200
C	0.07218300	0.08393800	-1.18370400
H	-0.26842400	-0.45160500	-2.06861100
H	-0.34232000	1.08964500	-1.23511100
H	1.16308300	0.16270600	-1.23258100

$(CH_3)_2$-NH (DMA)

N	0.00247600	-0.00465500	0.00247700
H	-0.00086200	0.00126600	1.01335200
C	1.36977800	-0.00010000	-0.48568500
H	1.36046100	0.12828200	-1.56902500
H	1.91584100	0.83728100	-0.05478100
H	1.91680400	-0.92757600	-0.26426800
C	-0.74910700	-1.14669500	-0.48604800
H	-0.27191300	-2.11200800	-0.26489700
H	-1.74889200	-1.14591900	-0.05529900
H	-0.85131600	-1.06842000	-1.56935800

OCS••NH_3 (TS1)

C	-0.11736900	-0.23180700	-0.34542900
S	1.27973400	-0.11946700	0.66944100
O	-1.29491500	-0.14828000	-0.21716000
N	0.53840700	-0.50957000	-1.69951000
H	0.23792600	-1.40686300	-2.07409600
H	1.60356000	-0.41556700	-0.89691000
H	0.31276600	0.21970200	-2.37258200

OCS••NH_3 (RC1)

C	-0.62126500	0.28849000	0.72700100
S	0.60462500	-0.11390200	1.61083700
O	-1.53754800	0.59367200	0.10397700
N	0.37132100	-0.47917200	-2.09197200
H	0.23114800	-1.44611300	-2.35694400
H	1.17644400	-0.14386200	-2.60564100
H	-0.43370700	0.03977100	-2.42075100

OCS••NH_3 (P1)

C	-0.50806000	0.06834800	-0.28123900
S	0.88912800	-0.06016200	0.85317800
O	-1.58998700	0.46956300	0.05285900
N	-0.18901600	-0.32993400	-1.53631400
H	0.71557100	-0.69633300	-1.76808400
H	0.16719600	0.38162400	1.88885700
H	-0.91393600	-0.31347800	-2.23295700

OCS••MA (RC2)

C	-3.15576600	-0.75871400	-0.61917300
S	-3.55582800	0.17108500	0.57717700
O	-2.89546900	-1.43075900	-1.51200000
N	-0.22486900	-0.85609300	0.06252800
H	0.42274900	-1.62954500	-0.00785200

H	-0.05254600	-0.40414500	0.95081300
C	-0.03448700	0.08090600	-1.04179200
H	-0.23496100	-0.43165000	-1.98144000
H	-0.75954400	0.89023200	-0.95002600
H	0.96325300	0.52639400	-1.09959400

OCS••MA (TS2)

C	-0.13476800	-0.19652700	-0.38684300
S	1.20174200	-0.00367200	0.69814500
O	-1.32080500	-0.13723900	-0.31563200
N	0.58090000	-0.56726600	-1.67342200
H	1.61813500	-0.44573000	-0.78208500
H	0.48960300	0.20520100	-2.33014900
C	0.08464800	-1.82003300	-2.25607300
H	-0.99046600	-1.76465500	-2.42423500
H	0.60011300	-2.01475800	-3.19247500
H	0.29471200	-2.62624200	-1.55548500

OCS••MA (P2)

C	-0.42386000	0.65170100	-0.17449600
S	0.44754100	-0.12150300	1.20632400
O	-0.98416200	1.71453700	-0.08484000
N	-0.37671500	-0.08809700	-1.30273600
H	0.16987700	0.89626000	2.02811800
H	0.11247400	-0.96478500	-1.30145600
C	-1.03258600	0.38190800	-2.50856300
H	-0.62686900	1.34560600	-2.81219600
H	-0.86749800	-0.34414500	-3.29914200
H	-2.10244100	0.49817300	-2.34196600

OCS••DMA (TS3)

C	-0.17341000	-0.24481200	-0.39404000
S	1.18441000	-0.10561700	0.67494600
O	-1.35763800	-0.17949500	-0.29194800
N	0.50989100	-0.51111300	-1.71928600
H	1.58596700	-0.39231200	-0.82419200
C	0.22746300	0.56901300	-2.66746600
H	0.76724000	0.37873900	-3.59268400
H	-0.84401600	0.62540900	-2.87072900
H	0.56338300	1.51185900	-2.23875800
C	0.13192700	-1.82896400	-2.23494100
H	-0.94334300	-1.86981900	-2.42120400
H	0.67236900	-2.01584600	-3.16046100
H	0.39955100	-2.58581000	-1.49929800

OCS••DMA (RC3)

C	-0.91832900	1.89824900	1.61907800
S	-0.22869200	2.53258600	2.87327700

O	-1.43054900	1.47288700	0.68310600
N	-0.01951500	-0.91068500	1.97530100
H	0.13097900	-1.38062600	2.85756400
C	1.25568600	-0.54419400	1.38509200
H	1.07367500	0.07236900	0.50201100
H	1.83646100	0.04588600	2.09241300
H	1.85570900	-1.40779300	1.06731600
C	-0.81428900	-1.74566500	1.09164300
H	-0.28718100	-2.64879200	0.75451900
H	-1.73413100	-2.04448300	1.59135200
H	-1.08593100	-1.16555900	0.20860600

OCS••DMA (P3)

C	0.04697200	-0.51031200	0.44133800
S	0.76795600	0.93484200	1.26274800
O	-0.32822400	-1.46035300	1.08548800
N	-0.02035100	-0.41271200	-0.90863700
H	0.65043500	0.34939600	2.45947000
C	0.33417500	0.77803500	-1.65301500
H	0.63884300	0.47933300	-2.65479100
H	-0.50748900	1.47015000	-1.73632300
H	1.17382800	1.29135500	-1.19159800
C	-0.71095700	-1.45481600	-1.64851700
H	-1.64511800	-1.07048800	-2.06452500
H	-0.08043600	-1.80346300	-2.46679300
H	-0.92774800	-2.27860100	-0.97789600

OCS••NH_3 (TS4)

C	-0.48600800	-0.23108100	-0.07210400
S	1.12637300	-0.15230500	0.11068200
O	-1.31255300	-0.15803600	-1.03433300
N	-1.48085100	-0.44400400	1.06402100
H	-1.46358700	0.30647100	1.74769400
H	-1.35729000	-1.33621700	1.53265700
H	-2.10779500	-0.34209900	-0.02369500

OCS••NH_3 (P4)

C	-0.26617900	-0.02681300	0.01434100
S	1.36199900	-0.27288400	-0.12007400
O	-1.05029100	0.29646700	-1.02195600
N	-0.97867000	-0.11749000	1.14071300
H	-1.97011900	0.05078700	1.13056000
H	-0.50944400	-0.35338400	1.99504800
H	-0.48173800	0.34533100	-1.80041100

OCS••MA (TS5)

C	-0.47252000	-0.19167000	-0.03806300
S	1.12915300	-0.10017000	0.22389900

O	-1.24718400	-0.08108600	-1.04271800
N	-1.50600600	-0.50007300	1.02564100
H	-1.58540500	0.28724800	1.66367900
H	-2.07813300	-0.36862200	-0.11652600
C	-1.29946200	-1.75478500	1.75703500
H	-0.34840000	-1.71729300	2.28713300
H	-2.11803400	-1.90560300	2.45561800
H	-1.27606500	-2.57216400	1.04044000

OCS••MA (P5)

C	-0.04708100	0.48314800	-0.16428100
S	0.83310500	1.87520500	-0.33307500
O	-0.41651300	-0.28109100	-1.20656700
N	-0.48094100	-0.03190200	0.98377700
H	-1.01086200	-0.88649200	0.92722000
H	-0.07105400	0.14478600	-2.00059000
C	-0.23224600	0.58185700	2.27067200
H	-0.65969400	1.58310600	2.30256800
H	-0.68751400	-0.03598200	3.03935500
H	0.83873800	0.66287400	2.45087300

OCS••DMA (RC4)

C	0.64128100	0.53515100	-1.32750900
S	1.80110200	-0.36788700	-0.78473100
O	-0.17688600	1.22024900	-1.75021200
N	-1.32411100	-0.36444200	0.70388300
H	-2.30027900	-0.44619000	0.45427500
C	-1.09144000	0.88973800	1.39820200
H	-1.55904200	0.93404300	2.39116900
H	-0.01562600	1.02391300	1.53379900
H	-1.46163000	1.71975200	0.79858000
C	-0.90849300	-1.51258100	1.48857800
H	-1.37250200	-1.55314700	2.48363000
H	-1.14273000	-2.43225200	0.95513400
H	0.17358200	-1.47138900	1.62587000

OCS••DMA (TS6)

C	-0.43843500	-0.23828700	-0.01819200
S	1.17013300	-0.17488300	0.20554200
O	-1.22743600	-0.15182400	-1.01661100
N	-1.45744200	-0.44355600	1.08021300
H	-2.04649500	-0.32548300	-0.07758900
C	-1.47567900	0.65969600	2.04470600
H	-2.31511300	0.52230900	2.72297400
H	-0.53884000	0.66949600	2.60442700
H	-1.58536200	1.60081000	1.51047700
C	-1.33093000	-1.75135700	1.72919600
H	-2.17068900	-1.89289700	2.40619600

H	-1.33596700	-2.53021000	0.96996300
H	-0.39144500	-1.79353000	2.28295600

OCS••DMA (P6)

C	-0.06066300	-0.15509700	-0.62286600
S	1.02017400	-1.23797000	-1.28011100
O	-0.49516600	0.90756000	-1.32502700
N	-0.57945400	-0.22453900	0.60137600
H	-0.05665200	0.85176800	-2.18301400
C	-1.51848200	0.75223100	1.13309200
H	-1.72617300	1.51418800	0.39334600
H	-2.44894700	0.25424500	1.40808800
H	-1.09638500	1.22019000	2.02328400
C	-0.19829700	-1.32263600	1.47606400
H	-0.72569300	-1.20346900	2.41878400
H	-0.46062900	-2.27799000	1.02416000
H	0.87661400	-1.31535400	1.65058800

H_2O

O	-1.66768100	0.91508700	0.00000000
H	-0.70893700	0.95004200	0.00000000
H	-1.95476600	1.83050600	0.00000000

Formic acid (FA)

C	-0.08544200	0.25505600	0.30964700
H	0.43484700	-0.61043200	-0.11381400
O	0.43155600	1.11845200	0.95044200
O	-1.38673200	0.20525800	0.00373800
H	-1.81291200	0.98263900	0.39258300

OCS••NH_3••H_2O (PRC1)

C	-0.89117800	-0.12568400	0.16766100
S	0.12497500	0.86556200	1.04061200
O	-1.86341100	-0.78954900	0.31148600
N	-0.39257100	-0.19679100	-1.44302600
H	-1.02476600	-0.80599500	-1.95495100
H	0.58070200	-0.53363200	-1.47119900
H	-0.41308100	0.74581000	-1.82135000
O	2.33876600	-0.49922600	-0.90971300
H	2.04555700	-0.01264800	-0.11999000
H	2.95834200	-1.16595700	-0.60608500

OCS••NH_3••H_2O (TS7)

C	-1.23538000	0.21716100	-0.09972200
S	-0.12562000	0.61277200	1.26399000
O	-2.41778600	0.39392300	0.03874100
N	-0.65368300	-0.26254300	-1.22231800
H	-1.26928900	-0.50527300	-1.97997100
H	2.75305300	-1.50191400	-0.85610500

H	0.33603300	-0.43549700	-1.29532500
O	2.33236900	-0.67115100	-1.09065300
H	1.02414600	0.28740600	0.65463100
H	3.01207500	-0.13617400	-1.50756500

OCS••NH_3••H_2O (PC1)

C	0.05194700	-0.33116600	-0.37867200
S	1.13824300	0.53709400	0.65572700
O	-1.00053800	-0.84506800	-0.12601700
N	0.55073300	-0.46382700	-1.78272900
H	-0.08213400	-1.08240500	-2.28202200
H	1.92368600	-0.71190800	-1.65378200
H	0.52513600	0.45423800	-2.22003900
O	2.95405100	-0.55386500	-1.22201800
H	2.48132800	-0.01523300	-0.34684500
H	3.33891600	-1.37718400	-0.90046300

OCS••NH_3••H_2O (PRC2)

C	0.69544700	0.29917500	-1.04518500
S	1.97978000	0.21604000	-0.15126000
O	-0.23416600	0.36252900	-1.71458900
N	-0.98034600	-0.24434000	1.59661300
H	-0.43743000	0.54558100	1.92369800
H	-0.37132800	-1.05318700	1.62011200
H	-1.71981100	-0.40310200	2.27149900
O	-3.08848100	0.12127400	-0.42993600
H	-2.28439800	0.02086100	0.10281300
H	-2.77921900	0.26741900	-1.32530100

OCS••NH_3••H_2O (TS8)

C	-0.64632500	-0.20411600	-0.04057200
S	0.93798800	-0.62916200	0.04912100
O	-1.31690500	0.27007700	-0.99481500
N	-1.50165000	-0.40505900	1.18913300
H	-1.42946100	0.44001200	1.75262900
H	-1.10161300	-1.16045200	1.73523000
H	-2.71583600	-0.44924800	0.68907400
O	-3.50368500	-0.13274200	-0.14810200
H	-2.56697400	0.14029500	-0.75392100
H	-3.98188200	-0.86277700	-0.55055200

OCS••NH_3••H_2O (PC2)

C	0.53745100	0.13691000	0.10955600
S	2.18151100	0.24649100	0.05114200
O	-0.19795200	0.08343200	-1.00272900
N	-0.16722800	0.09492600	1.25900600
H	-1.17196600	0.02420200	1.26892300
H	0.34536700	0.12987100	2.12081100

H	-3.39295600	-0.89274100	-0.31544800
O	-2.89971600	-0.09179500	-0.11830600
H	-1.14608000	0.02158300	-0.80005900
H	-3.48975700	0.64200300	-0.31080600

OCS••NH_3••FA (PRC3)

C	-1.52277400	-0.24518900	0.07967900
S	-0.83739100	0.89162500	1.11536300
O	-2.33371000	-1.11367900	0.15329800
N	-0.95035200	-0.09389000	-1.41357000
H	-1.41542900	-0.77276500	-2.01259500
H	0.08272400	-0.24142900	-1.40067000
H	-1.13148400	0.85417500	-1.73292300
C	2.55998400	-0.07104300	-0.46176700
H	3.63839400	-0.22387300	-0.56275900
O	1.77874600	-0.43711500	-1.31516500
O	2.25622600	0.53227900	0.65176300
H	1.26870500	0.65303300	0.74161700

OCS••NH_3••FA (TS9)

C	0.07108900	-0.42251600	-0.28861100
S	0.78421100	0.45551200	1.01678000
O	-0.87975000	-1.14794200	-0.28734000
N	0.77484200	-0.23622000	-1.58527900
H	0.24788800	-0.72366300	-2.30633700
H	1.99176700	-0.65135500	-1.48596800
H	0.82593700	0.75504700	-1.80585600
C	3.87319500	-0.23925800	-0.69892200
H	4.95345600	-0.38841000	-0.77262800
O	3.15034700	-0.97266600	-1.41938800
O	3.47595300	0.65040700	0.08973700
H	2.31187300	0.61024900	0.40095400

OCS••NH_3••FA (PC3)

C	-1.57268000	-0.18962700	-0.10145600
S	-0.93519400	0.38368600	1.46728600
O	-2.59755900	-0.80836500	-0.14922500
N	-0.78871200	0.07005700	-1.21247600
H	-1.29125500	-0.05816000	-2.08030800
H	0.91672400	-0.97329000	-1.00027200
H	-0.17290200	0.87238100	-1.17548100
C	2.48050300	-0.01011800	-0.57282000
H	3.55544500	-0.16223900	-0.43537800
O	1.87364200	-1.14449300	-0.87319000
O	1.94016800	1.06057200	-0.46005900
H	0.18849400	0.95060700	0.99860900

OCS••NH_3••FA (PRC4)

C	1.14159000	0.04047400	-0.03159500
S	2.60486000	-0.71447800	-0.06748100
O	0.45265100	0.68593700	-0.79800900
N	0.42329100	-0.07249000	1.39351200
H	0.64260100	0.77202200	1.91737100
H	0.80172100	-0.87446900	1.88983400
H	-0.60832200	-0.12886900	1.25319100
C	-2.78633900	0.40695100	-0.16400200
H	-3.87046700	0.44544000	-0.30464600
O	-2.28741900	-0.06172900	0.83942300
O	-2.14197900	0.91215900	-1.17562200
H	-1.15429900	0.85254700	-1.03637700

OCS••NH_3••FA (TS10)

C	1.10683300	0.00439900	0.01472200
S	2.42134000	-0.96508900	0.00210700
O	0.63122000	0.59853600	-1.06511600
N	0.35269800	0.24061200	1.16408800
H	-0.01999700	1.18121000	1.23936800
H	0.83107100	-0.06639100	1.99880800
H	-1.36654200	-0.53961000	0.84427600
C	-2.70690900	0.37088000	-0.12401900
H	-3.77817100	0.33228300	-0.33945400
O	-2.32486400	-0.63586600	0.62808000
O	-1.98584700	1.24885500	-0.53845000
H	-0.26285400	0.97209600	-0.91448000

OCS••NH_3••FA (PC4)

C	-0.73891100	-0.28817900	-0.05038600
S	0.64764300	-1.15631200	-0.06310900
O	-1.30061400	0.37318600	-0.96687300
N	-1.51425200	-0.23527600	1.22520500
H	-1.51864100	0.72463000	1.56917900
H	-1.06128000	-0.83196100	1.91131800
H	-2.66188000	-0.52917100	1.00887600
C	-4.35607100	0.06923900	-0.14628100
H	-5.43999900	0.12038500	-0.28627900
O	-3.92218600	-0.70930300	0.73273200
O	-3.66025500	0.81154900	-0.88564400
H	-2.46642700	0.61646200	-0.88090300

OCS••MA••H_2O (PRC5)

C	-0.70034000	0.02296200	0.45381400
S	0.27074200	1.15870600	1.20962700
O	-1.60951400	-0.69476600	0.72513900
N	-0.26957000	-0.12843100	-1.13359600

H	0.70830900	-0.45244800	-1.12060000
H	-0.24628500	0.82307800	-1.49190900
O	2.48498400	-0.40109100	-0.58417000
H	2.19237200	0.17287500	0.14532400
H	3.08282900	-1.04538100	-0.19926200
C	-1.15247300	-1.01026600	-1.91201700
H	-2.16193600	-0.61280000	-1.88441000
H	-0.79719200	-1.08009500	-2.93711400
H	-1.15512800	-1.98915900	-1.44428900

OCS••MA••H_2O (TS11)

C	0.06334200	-0.30390600	-0.34426000
S	1.17772900	0.63724300	0.60569700
O	-0.96073800	-0.82577000	-0.00595800
N	0.50621000	-0.48426600	-1.75389200
H	1.88259900	-0.75324500	-1.62157800
H	0.56276200	0.44571800	-2.16245100
O	2.92802300	-0.59559900	-1.23079400
H	2.46508800	0.01597800	-0.36716200
H	3.30023700	-1.40576200	-0.86497900
C	-0.36362900	-1.36069500	-2.54891900
H	-1.38981200	-1.00063100	-2.55176200
H	0.02150800	-1.40798100	-3.56456900
H	-0.35563400	-2.35432500	-2.11023500

OCS••MA••H_2O (PC5)

C	-0.91800600	0.13694100	0.13344500
S	0.40446300	0.72984900	1.23228400
O	-2.08350600	0.30198800	0.39398800
N	-0.44584900	-0.48106900	-0.96082400
H	2.70118000	-0.89540900	0.02841500
H	0.55298400	-0.57659500	-1.08591800
O	2.53755500	-0.52262100	-0.84273400
H	-0.47045000	1.22171000	2.11596000
H	2.79442800	0.40093700	-0.76987400
C	-1.37243300	-1.01281800	-1.94162500
H	-2.00254600	-0.22044700	-2.34339000
H	-0.80004500	-1.46251600	-2.74760500
H	-2.01881600	-1.76590200	-1.49263900

OCS••MA••H_2O (PRC6)

C	0.42341000	0.19369500	-0.39145800
S	1.87986200	0.94846200	-0.16213300
O	-0.19532300	-0.31342700	-1.29556400
N	-0.39626200	0.06629500	0.99917600
H	0.02768200	0.73145600	1.64000400
H	-1.37631500	0.29978500	0.80196900
O	-2.77261500	-0.36756400	-0.35931900

H	-2.06805700	-0.44665400	-1.02502800
H	-3.57720000	-0.12895000	-0.82249600
C	-0.31657200	-1.31876400	1.51037200
H	0.73135700	-1.55925200	1.66937900
H	-0.87490400	-1.40824500	2.43814100
H	-0.74516500	-1.97191800	0.75630500

OCS••MA••H_2O (TS12)

C	-0.55209900	-0.06751900	-0.01688000
S	1.02222600	0.36605800	0.14834900
O	-1.21889600	-0.32162800	-1.06175000
N	-1.37792800	-0.21943000	1.22921300
H	-1.08170000	0.50831500	1.87100600
H	-2.58761400	-0.18464300	0.76286500
O	-3.39508000	-0.22256400	-0.12775500
H	-2.41216300	-0.34300200	-0.79662200
H	-3.95913200	-0.99913400	-0.13242500
C	-1.14457300	-1.54272400	1.84683400
H	-0.09199900	-1.65876900	2.09711600
H	-1.75853900	-1.63372100	2.73955900
H	-1.43286200	-2.30999300	1.13076300

OCS••MA••H_2O (PC6)

C	0.36524900	0.53108000	-0.09952700
S	1.96242000	0.96202200	-0.19846300
O	-0.32942200	0.12347000	-1.19086400
N	-0.38957200	0.52936900	0.98811300
H	-1.35714900	0.24080900	0.88699900
H	-2.35375300	-0.36437600	-0.90480200
O	-2.95157000	-0.32207600	-0.14922800
H	0.28933400	0.16198600	-1.93097400
H	-3.50557700	-1.10357600	-0.19416800
C	0.11517800	0.93128500	2.28371600
H	0.47559200	1.95865000	2.24922500
H	-0.69297400	0.84951800	3.00466700
H	0.94378000	0.29124800	2.58425900

OCS••MA••FA (PRC7)

C	-1.47378100	-0.18896200	0.44179600
S	-0.36252200	0.33283900	1.59629400
O	-2.60399200	-0.58086900	0.47212600
N	-0.93003200	-0.10394600	-1.03673200
H	-1.52455500	-0.73074400	-1.57609800
H	0.05842700	-0.41407000	-1.08772300
C	2.68713800	-0.30691800	-0.67228000
H	3.73328300	-0.41602400	-0.97432100
O	1.77144900	-0.55384200	-1.42943500
O	2.57399000	0.10921000	0.55639300
H	1.60966600	0.18674700	0.82370800

C	-1.01248300	1.27767900	-1.56425800
H	-2.04332400	1.61481800	-1.49829800
H	-0.37557100	1.90175000	-0.94447500
H	-0.66783500	1.29250900	-2.59457500

OCS••MA••FA (TS13)

C	0.13960500	-0.32799400	-0.04163200
S	1.14159800	0.25364300	1.23924000
O	-0.94005700	-0.83643500	0.04109400
N	0.70161800	-0.17311000	-1.41245700
H	0.06263600	-0.68791600	-2.01559700
H	1.80769600	-0.63133000	-1.49141800
C	3.88830600	-0.30550200	-1.03774500
H	4.94338900	-0.46409600	-1.29037800
O	3.04697700	-0.99136800	-1.67036600
O	3.63384600	0.54350100	-0.15400400
H	2.44414300	0.43784100	0.43748800
C	0.80736300	1.23591100	-1.86462400
H	-0.15149100	1.73801400	-1.75930100
H	1.55723100	1.73785300	-1.26070600
H	1.12062500	1.23574700	-2.90539900

OCS••MA••FA (PC7)

C	-1.51749900	-0.51154100	0.00608800
S	-0.43061500	-0.00441400	1.38767800
O	-2.58287800	-1.03465100	0.20471500
N	-0.99867400	-0.19781400	-1.18825900
H	-0.03391100	0.10181000	-1.24768700
H	1.65641300	-0.93631200	0.80364300
C	2.76239800	-0.43281100	-0.64095200
H	3.79320700	-0.54529500	-0.99096000
O	2.57329400	-1.08358600	0.49230500
O	1.92839900	0.20441000	-1.22858800
H	-1.10791700	-0.74292200	2.27453600
C	-1.74056500	-0.50785700	-2.39676400
H	-1.85800000	-1.58426000	-2.52125000
H	-2.73091500	-0.05944500	-2.35071500
H	-1.19833000	-0.10154900	-3.24525500

OCS••MA••FA (PRC8)

C	1.04736900	-0.10954600	-0.27707500
S	2.56260400	-0.76660900	-0.25211500
O	0.32764000	0.40307000	-1.12000200
N	0.35872000	-0.09833000	1.13274700
H	0.85430300	-0.77332600	1.70944600
H	-0.63662300	-0.36162800	0.99938100
C	-2.88525900	0.17948000	-0.34117900
H	-3.97257800	0.23512500	-0.45109600

O	-2.36558900	-0.26542300	0.66257600
O	-2.26197700	0.63956100	-1.38671600
H	-1.26716800	0.56142300	-1.27968700
C	0.40704000	1.25746200	1.72618800
H	-0.09647700	1.93427300	1.04189600
H	-0.10074300	1.25385400	2.68645000
H	1.44879900	1.54470200	1.84032900

OCS••MA••FA (TS14)

C	-0.73324100	-0.29807900	-0.09326200
S	0.71377500	-1.05565500	-0.07714800
O	-1.32829200	0.27602000	-1.05858100
N	-1.49399400	-0.22112200	1.17701500
H	-1.03104900	-0.84629100	1.83086400
H	-2.61233800	-0.53534600	0.99780300
C	-4.37538600	0.09227700	-0.07362100
H	-5.46427600	0.16908000	-0.17327300
O	-3.93396900	-0.68133200	0.80919500
O	-3.68416700	0.79448600	-0.84955200
H	-2.41216600	0.53307200	-0.92478200
C	-1.53748900	1.15952500	1.72417600
H	-2.05751400	1.79429200	1.01209900
H	-2.08667400	1.13916700	2.66129800
H	-0.52437600	1.52197900	1.88171400

OCS••MA••FA (PC8)

C	1.12206700	-0.56213700	0.03690300
S	2.74558000	-0.84686800	-0.10635300
O	0.32374700	-0.47988300	-1.06685400
N	0.43173500	-0.38892900	1.14892800
H	-0.56852400	-0.21956900	1.07422800
H	-1.47514000	-0.16373900	-1.29690500
C	-3.00627900	0.15711400	-0.24155400
H	-4.07913900	0.34565900	-0.34322900
O	-2.43288500	0.00330300	-1.41872900
O	-2.44186000	0.10139000	0.82049500
H	0.90486700	-0.61894800	-1.82639000
C	1.05001400	-0.42977000	2.45773400
H	1.81634800	0.33998700	2.53951700
H	0.27730400	-0.26188500	3.20206600
H	1.52068400	-1.39778500	2.62467600

OCS••DMA••H_2O (PRC9)

C	-0.78308600	0.01853800	0.63107400
S	0.47431400	0.15930500	1.73079700
O	-1.97643000	0.07180600	0.66993200
N	-0.25574700	-0.21225000	-0.88628700
H	0.71778800	-0.53042300	-0.82703800
O	2.57874000	-0.34491600	-0.63478500

H	2.30169300	-0.14538400	0.27878000
H	3.32124100	-0.94901900	-0.57035100
C	-1.08499900	-1.21579000	-1.57498400
H	-2.11404900	-0.86955600	-1.56595500
H	-0.72908800	-1.33918800	-2.59565100
H	-1.01598300	-2.15661600	-1.03530300
C	-0.26253300	1.09458500	-1.57628900
H	0.39418800	1.76858000	-1.03285400
H	0.09395400	0.96846800	-2.59621300
H	-1.28191900	1.47307900	-1.57208800

OCS••DMA••H_2O (TS15)

C	0.06072300	-0.24898500	-0.33067200
S	1.29693600	0.32218500	0.75279600
O	-1.07561000	-0.51640200	-0.06009100
N	0.50656500	-0.41010400	-1.74970700
H	1.85682600	-0.69069700	-1.67253100
O	2.93748500	-0.59700100	-1.33375800
H	2.46708000	-0.12917800	-0.30135500
H	3.32462700	-1.45653600	-1.13994900
C	-0.32706300	-1.38592100	-2.46280900
H	-1.35864200	-1.04196000	-2.52608600
H	0.08092400	-1.51953500	-3.46292200
H	-0.31031600	-2.33318000	-1.93012200
C	0.47309900	0.90481800	-2.42463400
H	1.11834700	1.59724800	-1.89055200
H	0.83680300	0.78254600	-3.44303800
H	-0.54719100	1.29244700	-2.44415900

OCS••DMA••H_2O (PC9)

C	-0.77534500	-0.14999300	0.63237600
S	-0.23323900	1.27287600	1.61043200
O	-1.33321900	-1.08345600	1.15541700
N	-0.47082500	-0.07186500	-0.69169800
H	1.59897300	-0.92544100	-0.78449900
O	2.24245100	-0.96145700	-1.50019600
H	-0.68448700	0.70554700	2.73457300
H	2.96412200	-1.50483300	-1.17779000
C	-1.03832600	-1.07500400	-1.58450500
H	-1.92680600	-0.68235400	-2.08470200
H	-0.29238600	-1.34144000	-2.33179700
H	-1.31254900	-1.94998600	-1.00571900
C	-0.00070000	1.14734400	-1.32959200
H	0.72333400	1.65934700	-0.70060200
H	0.50827100	0.87067000	-2.25009700
H	-0.82748800	1.82394200	-1.55820900

OCS••DMA••H_2O (PRC10)

C	0.44324400	0.05867500	-0.62424700

S	2.07952300	0.03842800	-0.38703400
O	-0.31525100	0.24620000	-1.54519200
N	-0.42527200	-0.19667500	0.74426300
H	-1.37200700	-0.37630300	0.39297700
O	-2.88865300	0.16472400	-0.63112400
H	-2.19929900	0.27606700	-1.30696800
H	-3.68606700	-0.12215300	-1.07892000
C	0.04084800	-1.33770100	1.54955600
H	1.04803800	-1.12243900	1.89302400
H	-0.63517800	-1.47839600	2.39146600
H	0.05879600	-2.22687000	0.92543800
C	-0.46486700	1.05853300	1.52220200
H	-0.85588600	1.84611500	0.88336700
H	-1.11121000	0.92847100	2.38801800
H	0.55068300	1.29296200	1.83072200

OCS••DMA••H_2O (TS16)

C	-0.59072200	-0.15068300	-0.05370400
S	1.03759500	-0.32634700	-0.00496300
O	-1.31696800	0.20318300	-1.03502200
N	-1.41317100	-0.37824800	1.18527100
H	-2.59107300	-0.44768100	0.70177900
O	-3.46777900	-0.17662600	-0.10357800
H	-2.46052600	0.06918300	-0.77833400
H	-3.97330300	-0.92217800	-0.43411200
C	-1.00820900	-1.55304800	1.96835000
H	-0.00821900	-1.41187100	2.37362500
H	-1.72783300	-1.68471100	2.77463000
H	-1.00893000	-2.43037200	1.32671000
C	-1.38637200	0.85019200	2.00767100
H	-1.71642800	1.68892200	1.39893200
H	-2.06952600	0.72178900	2.84473700
H	-0.37332400	1.02732900	2.36819300

OCS••DMA••H_2O (PC10)

C	0.34006000	0.13911400	-0.42386000
S	0.76764300	-1.21963400	-1.31148500
O	0.25929400	1.33687200	-1.02282600
N	0.03649400	0.17364600	0.86630900
H	-1.70596800	-1.31672600	-0.81870300
O	-2.46759400	-0.98258500	-0.32394500
H	0.49743300	1.18957600	-1.94641500
H	-3.23308100	-1.16762000	-0.87130400
C	0.01160400	-1.04601300	1.65828000
H	0.78448900	-1.72320900	1.31233100
H	0.19126800	-0.77824400	2.69739900
H	-0.96311600	-1.52916900	1.56890500
C	-0.62268800	1.32265300	1.47369800
H	-0.44451700	2.21617800	0.88991000

H	-1.69616100	1.12844000	1.52727300
H	-0.23018600	1.46178200	2.47916100

OCS••DMA••FA (PRC11)

C	-1.43670500	0.05664500	0.46836800
S	-0.38125500	-0.09998300	1.77260600
O	-2.62681500	0.12787000	0.36041500
N	-0.70319600	0.12778500	-0.92780800
H	0.31311000	0.05373800	-0.77263600
C	2.90777200	-0.13910300	-0.24093200
H	3.97944400	-0.18675900	-0.45832600
O	2.07604000	-0.02647600	-1.11623100
O	2.66491600	-0.21725200	1.03748300
H	1.67924600	-0.17274100	1.21254600
C	-0.97982100	1.43109200	-1.56578800
H	-0.62922300	2.21808600	-0.90259900
H	-0.45103400	1.47895000	-2.51488900
H	-2.05266100	1.51797400	-1.71271300
C	-1.12683100	-1.00960000	-1.76966900
H	-0.59901000	-0.96154700	-2.71928900
H	-0.87794900	-1.93160400	-1.24999600
H	-2.20105300	-0.94341000	-1.91693500

OCS••DMA••FA (TS17)

C	0.02183300	-0.35716800	-0.20775700
S	0.92304800	0.13626000	1.18528200
O	-1.08593500	-0.80243000	-0.22026900
N	0.72905700	-0.19740700	-1.52002200
H	1.82211200	-0.57293000	-1.44761400
C	3.88777500	-0.20384200	-0.86864500
H	4.96769800	-0.31027900	-1.03811200
O	3.13209100	-0.92371500	-1.56931800
O	3.52077100	0.62188600	-0.00505800
H	2.23356300	0.40345000	0.52394400
C	0.83351600	1.23448600	-1.89673500
H	1.39404000	1.76561200	-1.13384300
H	1.36384700	1.29140400	-2.84445100
H	-0.16544400	1.65556500	-1.99887900
C	0.08011200	-0.98744000	-2.58560100
H	0.71077200	-0.92416900	-3.46909700
H	-0.00058300	-2.01949100	-2.25986200
H	-0.91282500	-0.59587500	-2.78994800

OCS••DMA••FA (PC11)

C	-1.28793100	-0.36413900	0.38195500
S	-0.93657600	0.72719000	1.76880500
O	-1.86730800	-1.40889300	0.52908300
N	-0.79139300	0.07152500	-0.82693300
H	0.97833500	-0.76509000	-0.65618500

C	2.77072600	-0.24565500	-0.39039700
H	3.77615300	-0.67868000	-0.35059200
O	1.86618800	-1.18227400	-0.65180500
O	2.53170900	0.91655800	-0.22348500
H	-1.49274200	-0.13711300	2.62598400
C	-0.46305200	1.47672500	-1.04791200
H	0.13800200	1.86434300	-0.23101900
H	0.14531300	1.54524700	-1.94714000
H	-1.36617100	2.07802900	-1.17527000
C	-1.26026000	-0.65106300	-2.00757200
H	-0.52497800	-0.53138000	-2.80106700
H	-1.37182200	-1.70222300	-1.76452600
H	-2.22204400	-0.26047900	-2.34854600

OCS••DMA••FA (PRC12)

C	0.98435300	0.07797200	-0.46844300
S	2.63403300	0.00307300	-0.45923100
O	0.13238000	0.12728200	-1.34179000
N	0.30394400	0.10918800	0.96213300
H	-0.71190300	0.09456200	0.76313100
C	-3.04938500	0.15146500	-0.45730300
H	-4.14097200	0.16670200	-0.53409500
O	-2.48121500	0.12035100	0.61543600
O	-2.47410300	0.17084000	-1.62508100
H	-1.47808900	0.15543200	-1.52690300
C	0.61210800	1.36917700	1.67057700
H	0.34078900	2.20310300	1.02826800
H	0.03408200	1.40354600	2.59170000
H	1.67848700	1.39247400	1.87587800
C	0.63805400	-1.07809900	1.77440800
H	0.39313200	-1.97023900	1.20422100
H	1.70301400	-1.05919600	1.98565100
H	0.05393400	-1.04725500	2.69194500

OCS••DMA••FA (TS18)

C	-0.67933100	-0.24891800	-0.11771800
S	0.82758100	-0.86367500	-0.20252800
O	-1.34340700	0.28349400	-1.07409500
N	-1.42794300	-0.21502600	1.16437100
H	-2.55799200	-0.50460600	0.96504700
C	-4.36789400	0.05063700	0.00819000
H	-5.46289300	0.08678200	-0.04365800
O	-3.86540300	-0.71068700	0.87678500
O	-3.72740900	0.76737800	-0.78816100
H	-2.39011400	0.50883800	-0.90670300
C	-1.48256600	1.18130600	1.67083100
H	-1.90806100	1.82363900	0.90517000
H	-2.11908200	1.19429900	2.55224600
H	-0.47538100	1.50844400	1.92479800

C	-0.94853300	-1.13594700	2.21077700
H	-0.89226600	-2.13933800	1.80196800
H	0.03586900	-0.83342700	2.55797300
H	-1.67304800	-1.10248900	3.02220200

OCS••DMA••FA (PC12)

C	0.81944900	0.09922200	-0.35363200
S	0.82379000	-1.48534100	-0.93264700
O	0.87882600	1.12326300	-1.21359000
N	0.76725300	0.46466300	0.91340700
H	-1.45105400	-1.50434300	-0.78588700
C	-2.85375600	-0.43904000	-0.08063900
H	-3.94861100	-0.38932400	-0.07518500
O	-2.43628800	-1.47960700	-0.77662600
O	-2.15111900	0.35840000	0.48144200
H	0.92486000	0.73334100	-2.09538700
C	0.54498400	1.84807300	1.31820900
H	0.76847300	2.52141900	0.50125000
H	-0.49842300	1.96587900	1.61314000
H	1.19300900	2.07351200	2.16333800
C	0.59441300	-0.53073300	1.95905600
H	1.19200700	-1.40838700	1.73735900
H	0.91346600	-0.09117800	2.90102100
H	-0.45706400	-0.81487300	2.02708900

Table S6: The comparison of energies for the various complexes involved in the OCS + NH_3 + H_2O and OCS + DMA + FA reactions calculated at the M06-2X, M06-2X-D3, CCSD(T)//M06-2X, and CCSD(T)//M06-2X-D3 levels of theory. All the energies of the complexes were calculated relative to the energies of the corresponding OCS + NH_3 + H_2O and OCS + DMA + FA separated starting reactants.

Stationary point	M06-2X/ aug-cc-pVTZ	CCSD(T)/aug-cc-pVTZ// M06-2X/aug-cc-pVTZ	M06-2X-D3/ aug-cc-pVTZ	CCSD(T)/aug-cc-pVTZ// M06-2X-D3/aug-cc-pVTZ
PRC1	9.3	11.3	9.2	11.3
PC1	-4.5	-2.2	-4.6	-2.2
PRC2	-5.6	-5.8	-5.8	-5.8
PC2	1.3	5.3	1.2	5.3
PRC3	4.1	5.4	4.0	5.4
PC3	-6.7	-4.8	-6.8	-4.8
PRC4	3.9	5.3	3.9	5.3
PC4	1.0	2.0	-1.1	2.0

Table S7. Calculated equilibrium constants (cm^3 $molecule^{-1}$) for the formation of various dimer complexes.

T (K)	OCS••DMA ($K_{eq}1$)	OCS••H_2O ($K_{eq}10$)	OCS••H_2O ($K_{eq}11$)	OCS••FA ($K_{eq}12$)	OCS••FA ($K_{eq}13$)
200	4.04×10^{-23}	2.19×10^{-27}	2.45×10^{-29}	5.25×10^{-22}	2.18×10^{-22}
210	3.02×10^{-23}	1.71×10^{-27}	2.32×10^{-29}	2.26×10^{-22}	1.03×10^{-22}
220	2.34×10^{-23}	1.38×10^{-27}	2.22×10^{-29}	1.06×10^{-22}	5.22×10^{-23}
230	1.84×10^{-23}	1.12×10^{-27}	2.11×10^{-29}	5.26×10^{-23}	2.78×10^{-23}
240	1.50×10^{-23}	9.27×10^{-28}	2.02×10^{-29}	2.78×10^{-23}	1.58×10^{-23}
250	1.24×10^{-23}	7.82×10^{-28}	1.95×10^{-29}	1.55×10^{-23}	9.36×10^{-24}
260	1.05×10^{-23}	6.68×10^{-28}	1.88×10^{-29}	9.07×10^{-24}	5.79×10^{-24}
270	8.96×10^{-24}	5.79×10^{-28}	1.83×10^{-29}	5.25×10^{-24}	3.72×10^{-24}
280	7.79×10^{-24}	5.07×10^{-28}	1.78×10^{-29}	3.49×10^{-24}	2.47×10^{-24}
290	6.86×10^{-24}	4.48×10^{-28}	1.74×10^{-29}	2.28×10^{-24}	1.69×10^{-24}
298	6.23×10^{-24}	4.08×10^{-28}	1.71×10^{-29}	1.64×10^{-24}	1.26×10^{-24}
300	6.10×10^{-24}	4.00×10^{-28}	1.70×10^{-29}	1.53×10^{-24}	1.18×10^{-24}

Table S8. Calculated equilibrium constants (cm^3 $molecule^{-1}$) for the formation of various reactant complexes from the reaction of the corresponding dimer complex and a monomer.

T (K)	OCS••DMA (RC3) + H_2O <=> PRC9 ($^{K}eq2$)	OCS••H_2O (RC4) + DMA <=> PRC9 ($^{K}eq3$)	OCS••DMA (RC3) + H_2O <=> PRC10 ($^{K}eq4$)	OCS••H_2O (RC5) + DMA <=> PRC10 (K_{eq5})	OCS••DMA (RC3) + FA <=> PRC11 (K_{eq6})	OCS••FA (RC7) + DMA <=> PRC11 (K_{eq7})	OCS••DMA (RC3) + FA <=> PRC12 (K_{eq8})	OCS••FA (RC8) + DMA <=> PRC12 (K_{eq9})
200	1.38×10^{-27}	2.19×10^{-27}	1.64×10^{-29}	2.45×10^{-29}	2.40×10^{-21}	5.25×10^{-22}	1.14×10^{-21}	2.18×10^{-22}
210	1.32×10^{-27}	1.71×10^{-27}	1.86×10^{-29}	2.32×10^{-29}	1.05×10^{-21}	2.26×10^{-22}	5.15×10^{-22}	1.03×10^{-22}
220	1.27×10^{-27}	1.38×10^{-27}	2.09×10^{-29}	2.22×10^{-29}	4.96×10^{-22}	1.06×10^{-22}	2.50×10^{-22}	5.22×10^{-23}
230	1.22×10^{-27}	1.12×10^{-27}	2.31×10^{-29}	2.11×10^{-29}	2.50×10^{-22}	5.26×10^{-23}	1.30×10^{-22}	2.78×10^{-23}
240	1.18×10^{-27}	9.27×10^{-28}	2.55×10^{-29}	2.02×10^{-29}	1.34×10^{-22}	2.78×10^{-23}	7.11×10^{-23}	1.58×10^{-23}
250	1.14×10^{-27}	7.82×10^{-28}	2.78×10^{-29}	1.95×10^{-29}	7.55×10^{-23}	1.55×10^{-23}	4.09×10^{-23}	9.36×10^{-24}
260	1.11×10^{-27}	6.68×10^{-28}	3.02×10^{-29}	1.88×10^{-29}	4.45×10^{-23}	9.07×10^{-24}	2.46×10^{-23}	5.79×10^{-24}
270	1.09×10^{-27}	5.79×10^{-28}	3.26×10^{-29}	1.83×10^{-29}	2.73×10^{-23}	5.52×10^{-24}	1.54×10^{-23}	3.72×10^{-24}
280	1.06×10^{-27}	5.07×10^{-28}	3.50×10^{-29}	1.78×10^{-29}	1.74×10^{-23}	3.49×10^{-24}	9.96×10^{-24}	2.47×10^{-24}
290	1.04×10^{-27}	4.48×10^{-28}	3.75×10^{-29}	1.74×10^{-29}	1.14×10^{-23}	2.28×10^{-24}	6.65×10^{-24}	1.69×10^{-24}
298	1.03×10^{-27}	4.08×10^{-28}	3.96×10^{-29}	1.71×10^{-29}	8.30×10^{-24}	1.64×10^{-24}	4.89×10^{-24}	1.26×10^{-24}
300	1.02×10^{-27}	4.00×10^{-28}	4.00×10^{-29}	1.70×10^{-29}	7.74×10^{-24}	1.53×10^{-24}	4.57×10^{-24}	1.18×10^{-24}

Table S9. CVT/SCT calculated unimolecular rate coefficients (k_2, k_6, k_7, k_{15}, k_{16}, k_{17}) for the OCS + DMA reaction in the absence of a catalyst and in the presence of a single water and a single formic acid molecule, computed at the CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ level.

T (K)	OCS + DMA (k_2)	OCS + DMA (k_6)	OCS + DMA + H_2O (k_7)	OCS + DMA + H_2O (k_{15})	OCS + DMA + FA (k_{16})	OCS + DMA +FA (k_{17})
200	3.98×10^{-14}	1.39×10^{-20}	8.35×10^{-1}	1.46×10^{-1}	1.24×10^{6}	6.20×10^{5}
210	2.53×10^{-13}	1.10×10^{-19}	1.92×10^{0}	4.11×10^{-1}	1.94×10^{6}	9.70×10^{5}
220	1.44×10^{-12}	9.50×10^{-19}	4.18×10^{0}	1.07×10^{0}	2.93×10^{6}	1.47×10^{6}
230	7.40×10^{-12}	7.33×10^{-18}	8.66×10^{0}	2.59×10^{0}	4.30×10^{6}	2.15×10^{6}
240	3.48×10^{-11}	5.01×10^{-17}	1.72×10^{1}	5.91×10^{0}	6.14×10^{6}	3.07×10^{6}
250	1.51×10^{-10}	3.06×10^{-16}	3.27×10^{1}	1.28×10^{1}	8.57×10^{6}	4.29×10^{6}
260	6.08×10^{-10}	1.69×10^{-15}	6.01×10^{1}	2.62×10^{1}	1.17×10^{7}	5.85×10^{6}
270	2.29×10^{-9}	8.55×10^{-15}	1.07×10^{2}	5.13×10^{1}	1.57×10^{7}	7.85×10^{6}
280	8.13×10^{-9}	3.97×10^{-14}	1.84×10^{2}	9.65×10^{1}	2.06×10^{7}	1.03×10^{7}
290	2.72×10^{-8}	1.71×10^{-13}	3.09×10^{2}	1.75×10^{2}	2.67×10^{7}	1.34×10^{7}
298	7.01×10^{-8}	5.34×10^{-13}	4.62×10^{2}	2.76×10^{2}	3.26×10^{7}	1.63×10^{7}
300	8.65×10^{-8}	6.88×10^{-13}	5.05×10^{2}	3.05×10^{2}	3.40×10^{7}	1.70×10^{7}

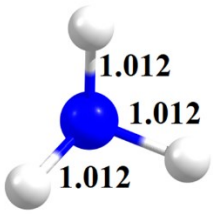
Table S10. The calculated effective first order rate coefficients (in s^{-1}) for the OCS + DMA (k_{TS3}^{eff}), OCS••DMA + H_2O (k_5^{eff}), OCS••H_2O + DMA (k_6^{eff}) reaction paths that proceed via H-atom transfer to the S-atom of OCS, and the OCS••DMA + H_2O (k_8^{eff}), OCS••H_2O + DMA (k_9^{eff}) reaction paths that proceed via H-atom transfer to the O-atom of OCS respectively, to form the corresponding carbamothioic acid.

T(K)	k_{TS3}^{eff}	$[H_2O]^a$	k_5^{eff}	k_6^{eff}	$k_{TS15}^{eff} = k_5^{eff} + k_6^{eff}$	k_8^{eff}	k_9^{eff}	$k_{TS16}^{eff} = k_8^{eff} + k_9^{eff}$
200	3.22×10^{-28}	1.09×10^{14}	1.02×10^{-27}	8.73×10^{-32}	1.02×10^{-27}	2.11×10^{-30}	1.91×10^{-36}	2.11×10^{-30}
210	1.53×10^{-27}	6.00×10^{14}	9.19×10^{-27}	6.75×10^{-31}	9.19×10^{-27}	2.77×10^{-29}	2.65×10^{-35}	2.77×10^{-29}
220	6.74×10^{-27}	1.15×10^{15}	2.85×10^{-26}	1.82×10^{-30}	2.85×10^{-26}	1.20×10^{-28}	1.21×10^{-34}	1.20×10^{-28}
230	2.73×10^{-26}	5.80×10^{-15}	2.26×10^{-25}	1.25×10^{-29}	2.26×10^{-25}	1.28×10^{-27}	1.33×10^{-33}	1.28×10^{-27}
240	1.04×10^{-25}	8.29×10^{15}	5.03×10^{-25}	2.45×10^{-29}	5.03×10^{-25}	3.73×10^{-27}	4.00×10^{-33}	3.73×10^{-27}
250	3.74×10^{-25}	2.21×10^{16}	2.05×10^{-24}	8.83×10^{-29}	2.05×10^{-24}	1.95×10^{-26}	2.15×10^{-32}	1.95×10^{-26}
260	1.27×10^{-24}	6.00×10^{16}	8.38×10^{-24}	3.22×10^{-28}	8.38×10^{-24}	9.92×10^{-26}	1.11×10^{-31}	9.92×10^{-26}
270	4.10×10^{-24}	1.50×10^{17}	3.12×10^{-23}	1.07×10^{-27}	3.12×10^{-23}	4.50×10^{-25}	5.14×10^{-31}	4.50×10^{-25}
280	1.27×10^{-23}	2.70×10^{17}	8.21×10^{-23}	2.55×10^{-27}	8.21×10^{-23}	1.42×10^{-24}	1.65×10^{-30}	1.42×10^{-24}
290	3.73×10^{-23}	5.20×10^{17}	2.29×10^{-22}	6.45×10^{-27}	2.29×10^{-22}	4.68×10^{-24}	5.49×10^{-30}	4.68×10^{-24}
298	8.74×10^{-23}	7.64×10^{17}	4.51×10^{-22}	1.18×10^{-26}	4.51×10^{-22}	1.04×10^{-23}	1.23×10^{-29}	1.04×10^{-23}
300	1.06×10^{-22}	8.24×10^{17}	5.20×10^{-22}	1.33×10^{-26}	5.20×10^{-22}	1.23×10^{-23}	1.45×10^{-29}	1.23×10^{-23}

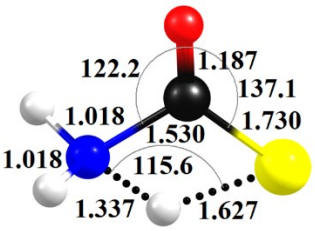
[a]Values of water concentration calculated based on using a typical temperature-dependent water concentration, which corresponds to 10%–100% relative humidity.

Table S11. The calculated effective first order rate coefficients (in s^{-1}) for the OCS + DMA (k_{TS6}^{eff}), OCS••DMA + FA (k_{10}^{eff}), OCS••FA + DMA (k_{11}^{eff}) reaction paths that proceed via H-atom transfer to the S-atom of OCS, and the OCS••DMA + FA (k_{13}^{eff}), OCS••FA + DMA (k_{14}^{eff}) reaction paths that proceed via H-atom transfer to the O-atom of OCS respectively, to form the corresponding carbamothioic acid.

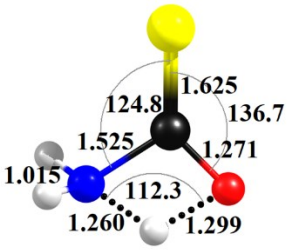
T(K)	k_{TS6}^{eff}	k_{10}^{eff}	k_{11}^{eff}	$k_{TS17}^{eff} = k_{10}^{eff} + k_{11}^{eff}$	k_{13}^{eff}	k_{14}^{eff}	$k_{TS18}^{eff} = k_{13}^{eff} + k_{14}^{eff}$
200	1.12×10^{-34}	1.20×10^{-17}	3.41×10^{-17}	4.62×10^{-17}	2.85×10^{-18}	2.95×10^{-18}	5.81×10^{-18}
210	6.64×10^{-34}	6.16×10^{-18}	9.93×10^{-18}	1.61×10^{-17}	1.51×10^{-18}	1.02×10^{-18}	2.53×10^{-18}
220	4.45×10^{-33}	3.40×10^{-18}	3.29×10^{-18}	6.69×10^{-18}	8.58×10^{-19}	3.98×10^{-19}	1.26×10^{-18}
230	2.70×10^{-32}	1.99×10^{-18}	1.19×10^{-18}	3.18×10^{-18}	5.14×10^{-19}	1.67×10^{-19}	6.81×10^{-19}
240	1.50×10^{-31}	1.23×10^{-18}	4.76×10^{-19}	1.71×10^{-18}	3.27×10^{-19}	7.63×10^{-20}	4.03×10^{-19}
250	7.58×10^{-31}	8.02×10^{-19}	2.07×10^{-19}	1.01×10^{-18}	2.17×10^{-19}	3.75×10^{-20}	2.55×10^{-19}
260	3.53×10^{-30}	5.44×10^{-19}	9.63×10^{-20}	6.41×10^{-19}	1.51×10^{-19}	1.96×10^{-20}	1.70×10^{-19}
270	1.53×10^{-29}	3.84×10^{-19}	4.79×10^{-20}	4.32×10^{-19}	1.08×10^{-19}	1.08×10^{-20}	1.19×10^{-19}
280	6.18×10^{-29}	2.79×10^{-19}	2.51×10^{-20}	3.04×10^{-19}	7.99×10^{-20}	6.26×10^{-21}	8.62×10^{-20}
290	2.34×10^{-28}	2.09×10^{-19}	1.38×10^{-20}	2.23×10^{-19}	6.09×10^{-20}	3.79×10^{-21}	6.47×10^{-20}
298	6.66×10^{-28}	1.69×10^{-19}	8.81×10^{-21}	1.77×10^{-19}	4.96×10^{-20}	2.59×10^{-21}	5.22×10^{-20}
300	8.40×10^{-28}	1.61×10^{-19}	7.97×10^{-21}	1.69×10^{-19}	4.74×10^{-20}	2.38×10^{-21}	4.98×10^{-20}



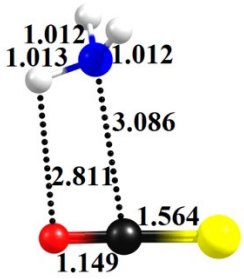
NH_3



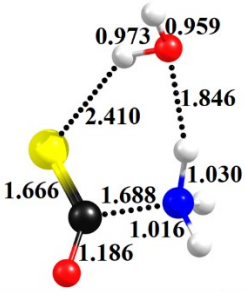
TS1



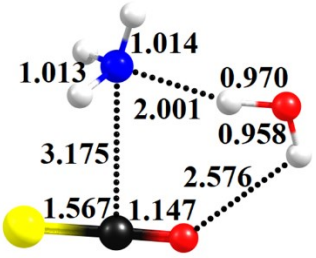
TS4



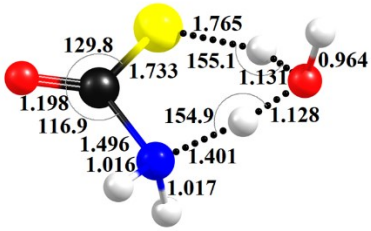
RC1



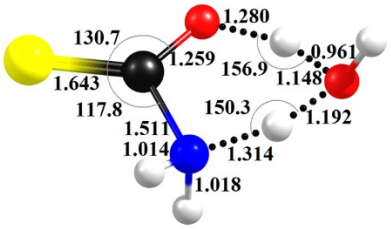
PRC1



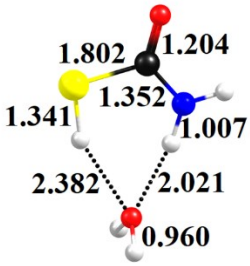
PRC2



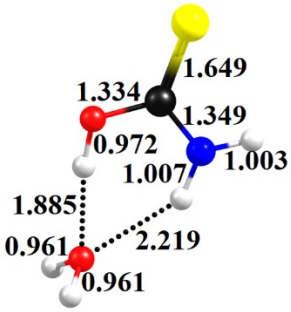
TS7



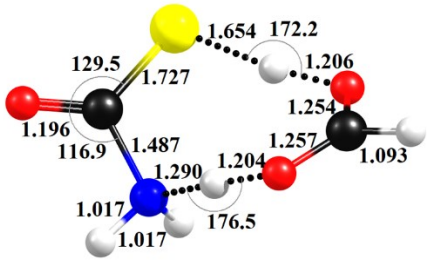
TS8



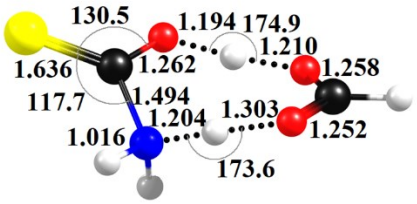
PC1



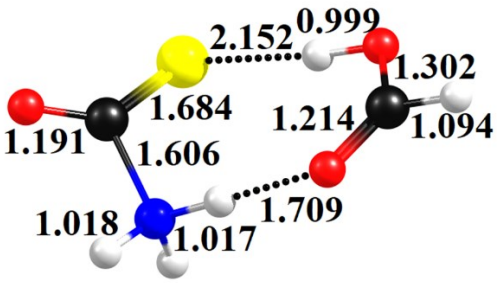
PC2



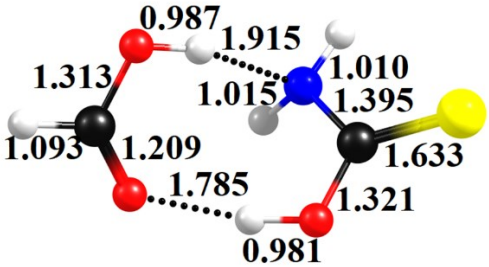
TS9



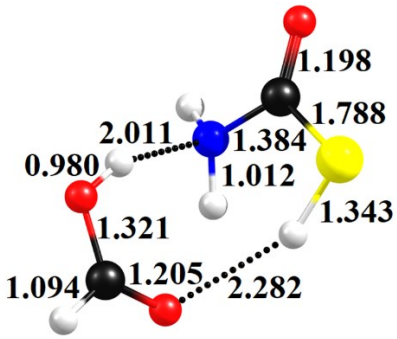
TS10



PRC3



PRC4



PC3

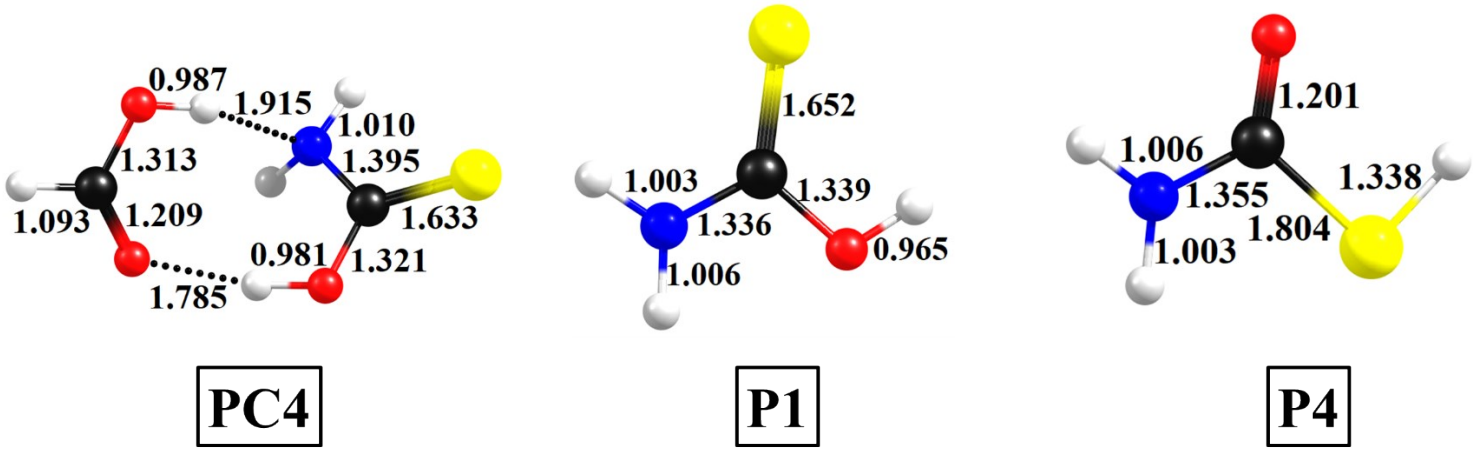
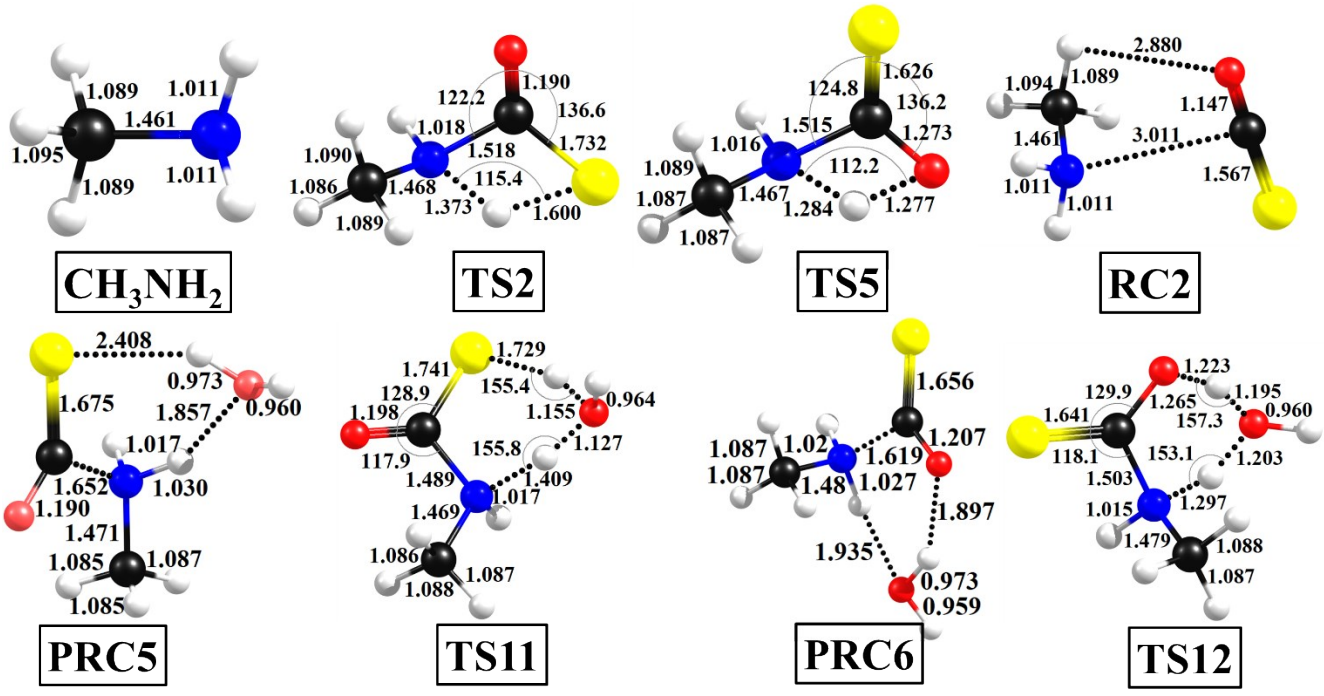


Figure S1. The M06-2X/aug-cc-pVTZ optimized geometries for the addition of ammonia to OCS without a catalyst and assisted by a water and a formic acid, leading to the formation of carbamothioic acid. The yellow, black, white, blue, and red colors represent sulfur, carbon, hydrogen, nitrogen, and oxygen atoms, respectively.



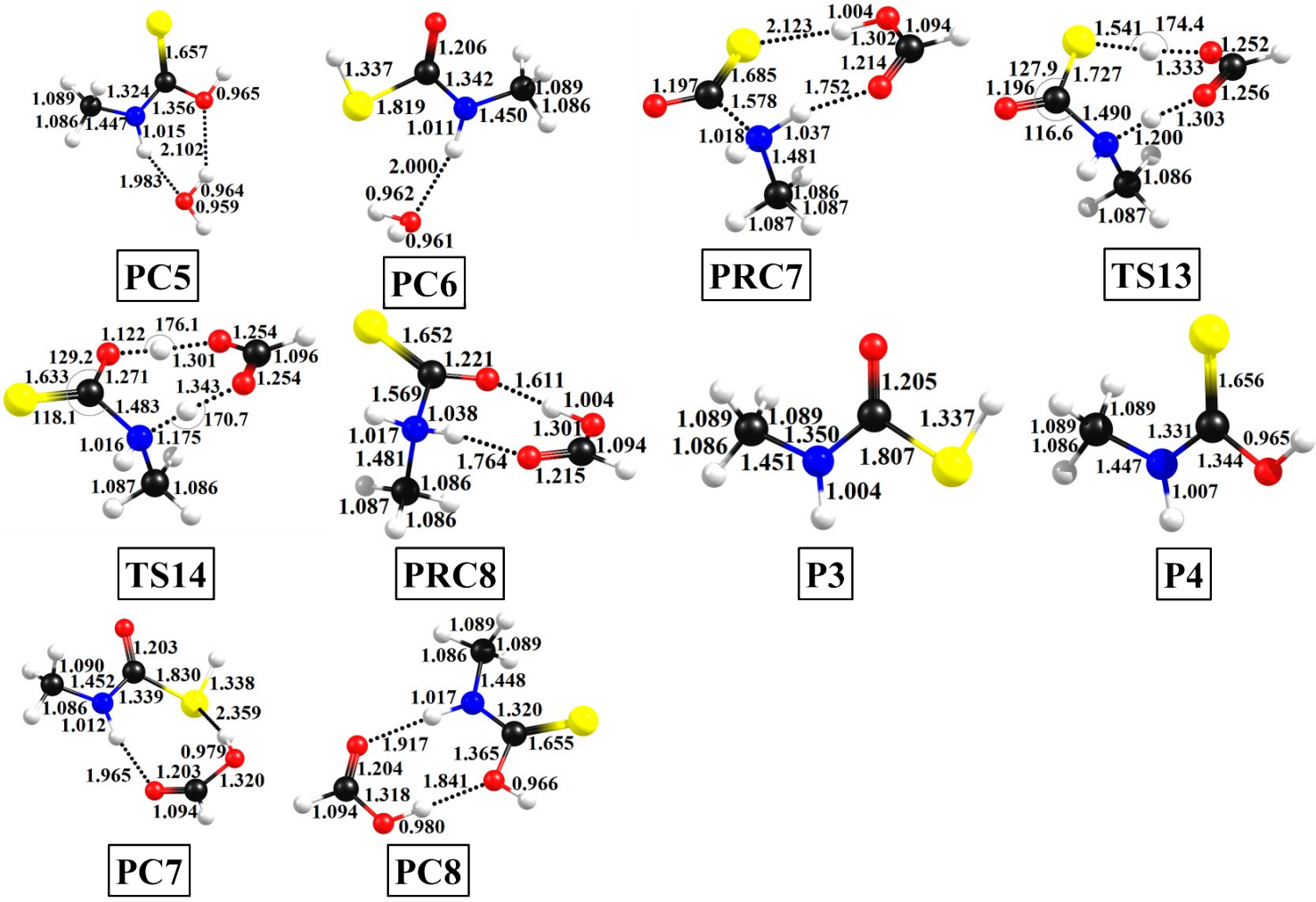


Figure S2. The M06-2X/aug-cc-pVTZ optimized geometries for the addition of methyl amine to OCS without a catalyst and assisted by a water and a formic acid, leading to the formation of *N*-methyl carbamothioic acid. The yellow, black, white, blue, and red colors represent sulfur, carbon, hydrogen, nitrogen, and oxygen atoms, respectively.

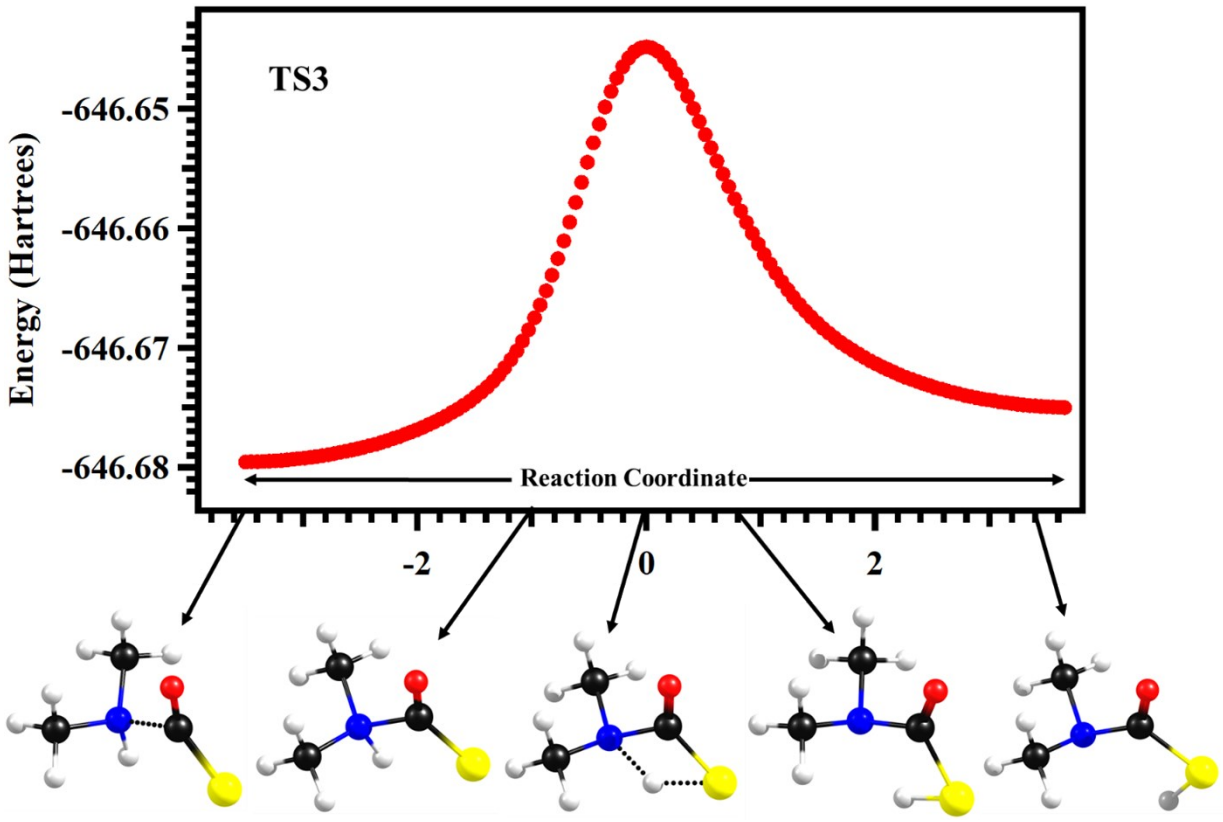


Figure S3. The M06-2X/aug-cc-pVTZ level calculated internal reaction coordinate (IRC) plot for the transition state (TS3) involving the OCS + DMA reaction in the absence of a catalyst. The reaction proceeds from a pre-reactive complex to a post-reactive complex via a transition state that is presented with the various indicated structures (see left to right) on the reaction coordinate. The yellow, black, white, blue, and red colors represent sulfur, carbon, hydrogen, nitrogen, and oxygen atoms, respectively.

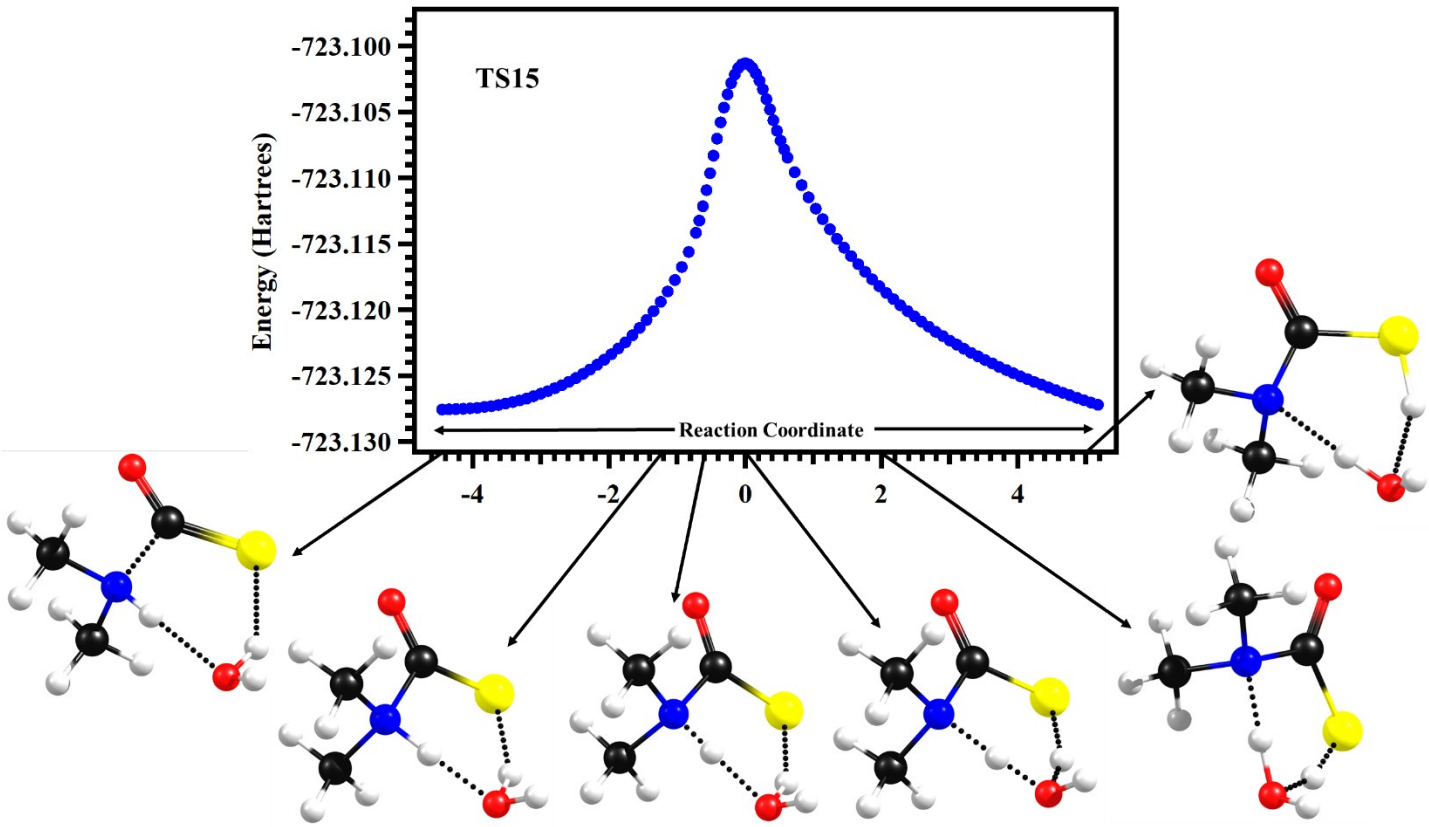


Figure S4. The M06-2X/aug-cc-pVTZ level calculated internal reaction coordinate (IRC) plot for the transition state (TS15) involving the OCS + DMA + H_2O reaction. The reaction proceeds from a pre-reactive complex to a post-reactive complex via a transition state that is shown with the various indicated structures (see left to right) on the reaction coordinate. The yellow, black, white, blue, and red colors represent sulfur, carbon, hydrogen, nitrogen, and oxygen atoms, respectively.

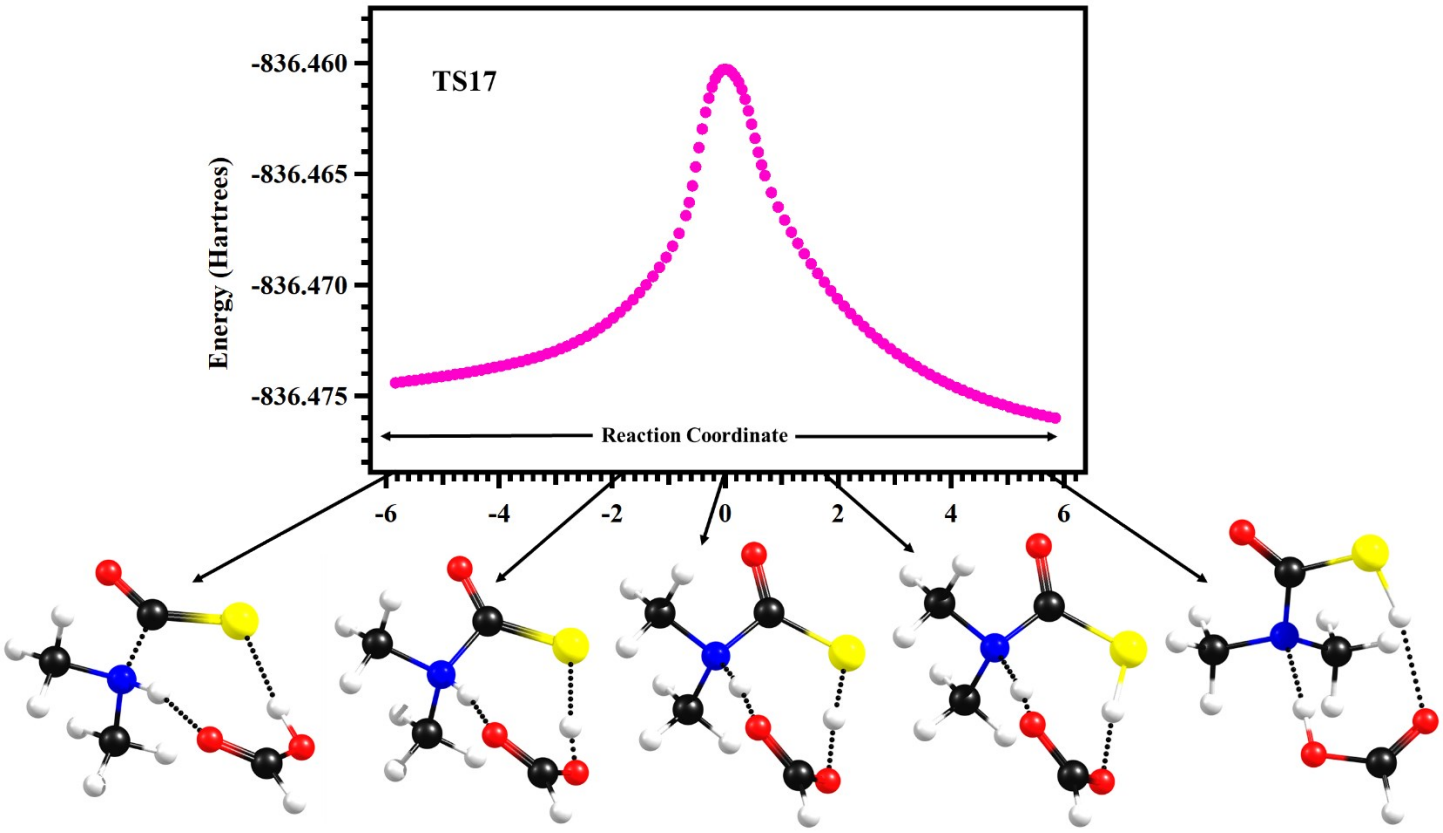


Figure S5. The M06-2X/aug-cc-pVTZ level calculated internal reaction coordinate (IRC) plot for the transition state (TS17) involving the OCS + DMA + FA reaction. The reaction proceeds from a pre-reactive complex to a post-reactive complex via a transition state that is shown with the various indicated structures (see left to right) on the reaction coordinate. The yellow, black, white, blue, and red colors represent sulfur, carbon, hydrogen, nitrogen, and oxygen atoms, respectively.

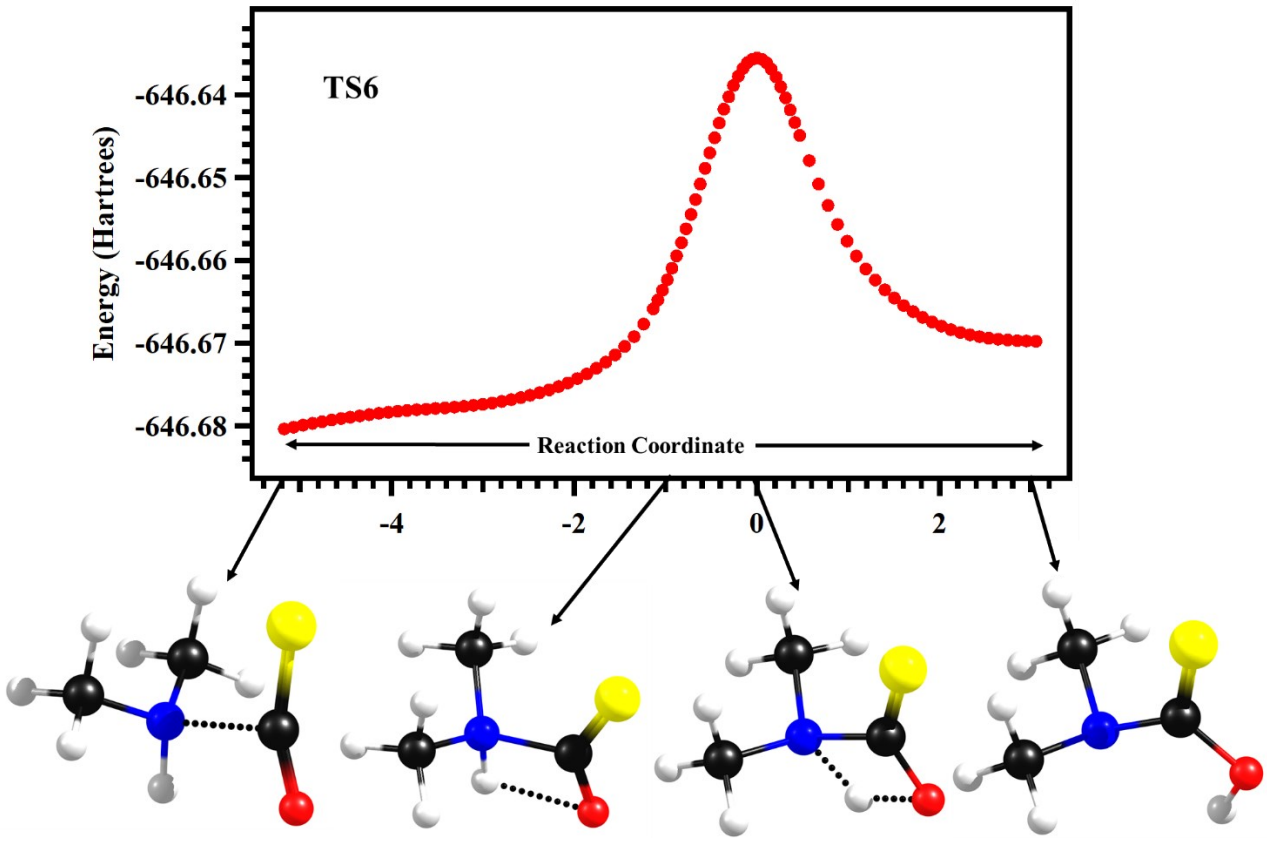


Figure S6. The M06-2X/aug-cc-pVTZ level calculated internal reaction coordinate (IRC) plot for the transition state (TS6) involving the OCS + DMA reaction in the absence of a catalyst. The reaction proceeds from a pre-reactive complex to a post-reactive complex via a transition state that is shown with the various indicated structures (see left to right) on the reaction coordinate. The yellow, black, white, blue, and red colors represent sulfur, carbon, hydrogen, nitrogen, and oxygen atoms, respectively.

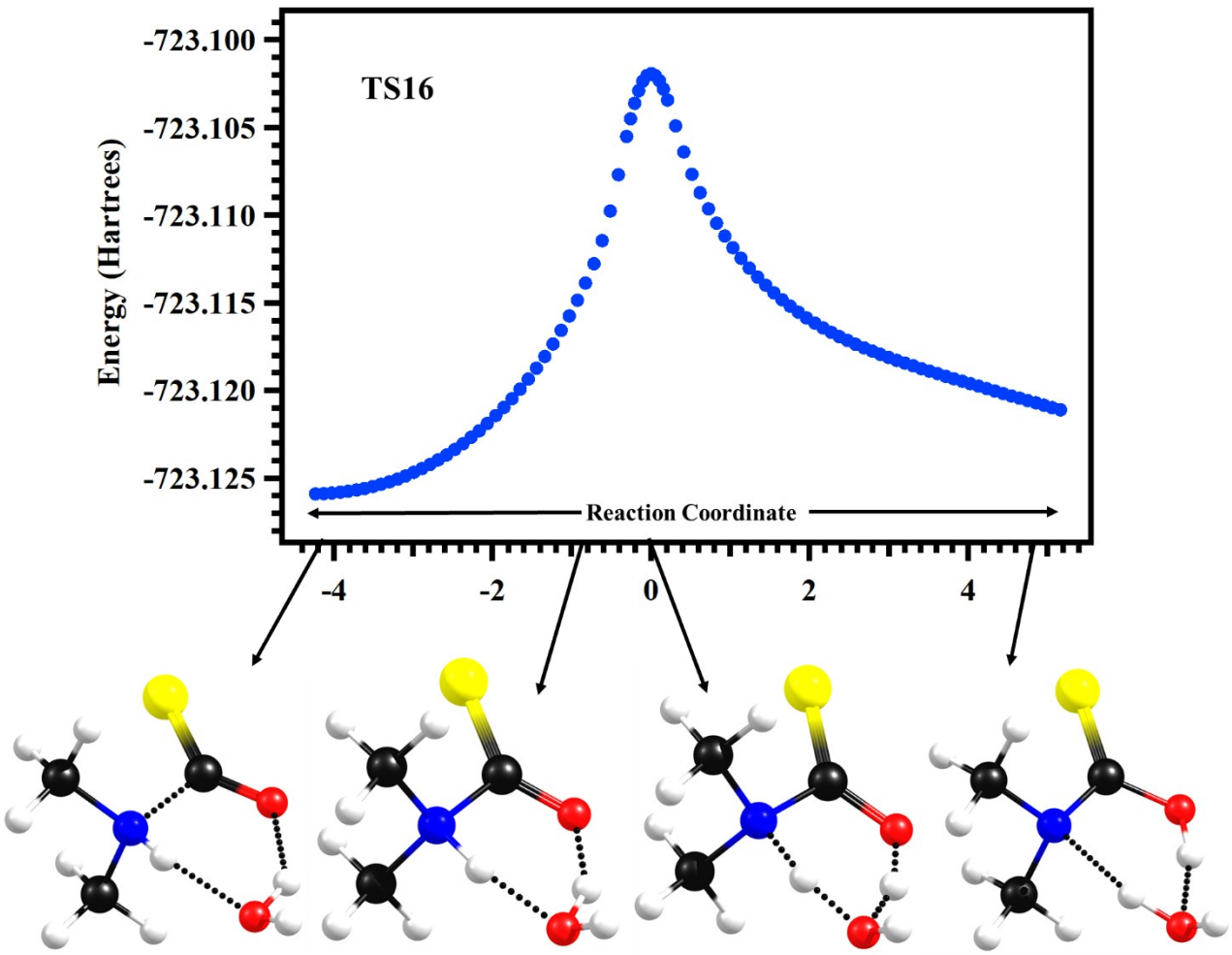


Figure S7. The M06-2X/aug-cc-pVTZ level calculated internal reaction coordinate (IRC) plot for the transition state (TS16) involving the OCS + DMA + H_2O reaction. The reaction proceeds from a pre-reactive complex to a post-reactive complex via a transition state that is shown with the various indicated structures (see left to right) on the reaction coordinate. The yellow, black, white, blue, and red colors represent sulfur, carbon, hydrogen, nitrogen, and oxygen atoms, respectively.

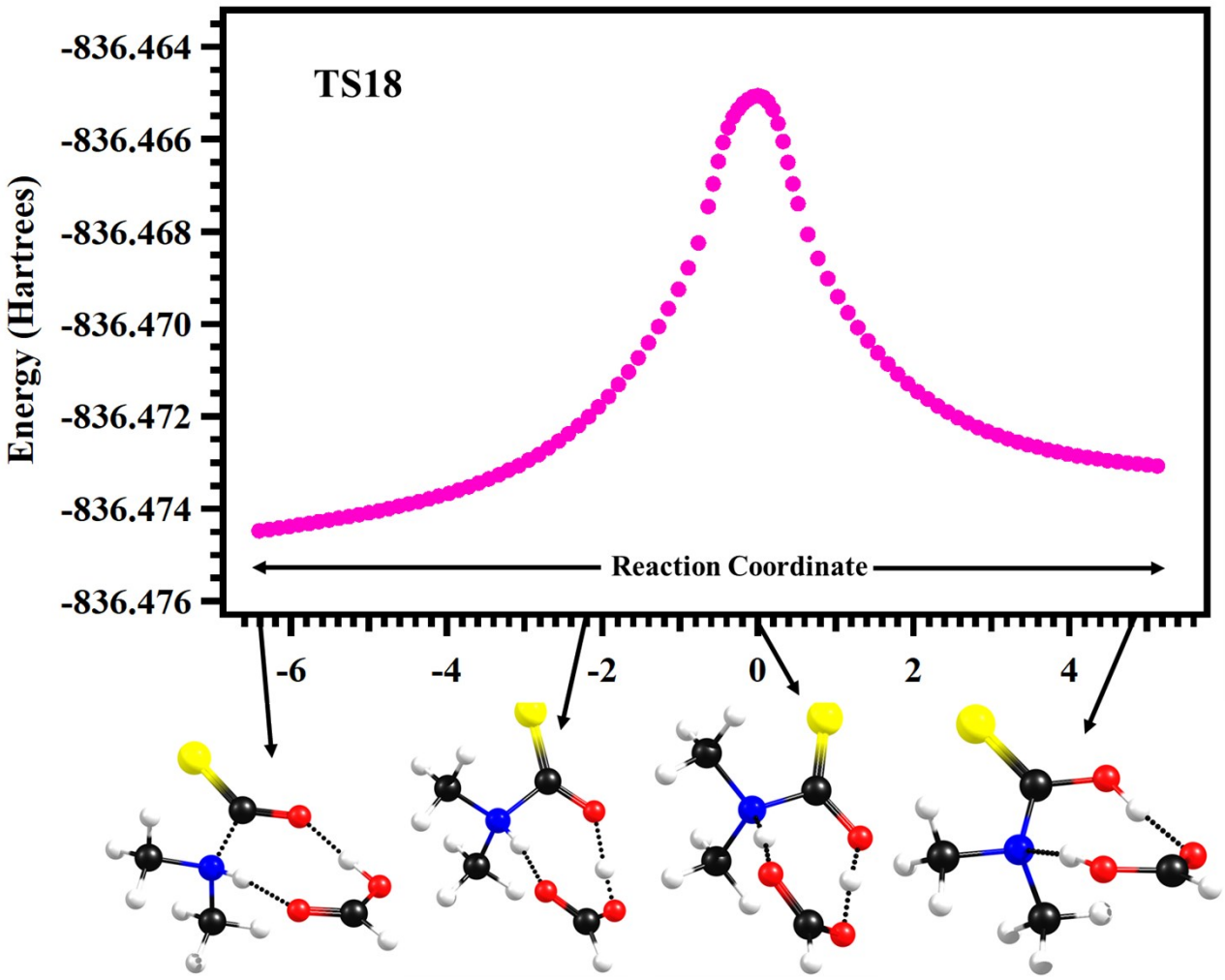


Figure S8. The M06-2X/aug-cc-pVTZ level calculated internal reaction coordinate (IRC) plot for the transition state (TS18) involving the OCS + DMA + FA reaction. The reaction proceeds from a pre-reactive complex to a post-reactive complex via a transition state that is shown with the various indicated structures (see left to right) on the reaction coordinate. The yellow, black, white, blue, and red colors represent sulfur, carbon, hydrogen, nitrogen, and oxygen atoms, respectively.