Appendix A. Supplementary data:

Can Silica Particles Reduce Air Pollution by Facilitating the Reactions of Aliphatic Aldehyde and NO_2?

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Methods. The rate constant can be obtained by variationally minimizing the generalized transition-state theory rate constant $k^{GT}(T,s)$ with respect to the dividing surface at s, that is,

$$k^{CVT}(T) = \min_{s} k^{GT}(T,s) \quad (1)$$

where

$$k^{GT}(T,s) = \frac{\sigma}{h\beta}\frac{Q^{GT}(T,s)}{Q^{R}(T)}\exp[-\beta V_{MEP}(s)] \quad (2)$$

In the equations (1) and (2), s is the location of the generalized transition state on IRC; σ is the symmetry factor accounting for possibility of two or more symmetry-related reaction paths; β equals $(k_B T)^{-1}$ where k_B is Boltzmann's constant, h is Planck's constant; $Q^R(T)$ is the reactant's partition function per unit volume, excluding symmetry numbers for rotation; $V_{MEP}(s)$ is the classical energy along the minimum-energy path (MEP) overall zero energy at the reactants; $Q^{GT}(T,s)$ is the partition function of generalized transition state at s with the local zero energy at $V_{MEP}(s)$ and with all rotational symmetry numbers set to unity.

Adsorption of aldehydes onto surface model. From Table S1, the E_{ae}s of $ADCI_{\text{-Monomer}}^{\text{-Acetaldehyde}}$, $ADCI_{\text{-Trimer}}^{\text{-Acetaldehyde}}$, and $ADCI_{\text{-Hexamer}}^{\text{-Acetaldehyde}}$ are calculated to be –6.22, –7.88, and –7.14 kcal mol^{-1}, respectively. Although there are some differences among them, the outside H atom that is free to be attacked by NO_2 is similar for three surface models. Therefore, it can be hopefully assumed that the slight increase in the adsorption energy did not affect significantly the energy barriers of the heterogeneous reaction. Increasing the model size of SiO_2 requires significantly the computational time. For example, for $ADCI_{\text{-Hexamer}}^{\text{-Acetaldehyde}}$, the CPU time of the geometry and energy calculations at the MPWB1K method required approximately 5040 and 1320 min on our workstation, respectively, while the corresponding computing times were only about 43 and 57 min for $ADCI_{\text{-Monomer}}^{\text{-Acetaldehyde}}$. As such, in this study, the monomer $Si(OH)_4$ was employed as the surface model to investigate the following heterogeneous reaction.

Table S1 The adsorption energies of the aldehyde onto the surface models (in kcal mol^{-1}).

	The monomer		The trimer		The hexamer	
	*ADC*1	*ADC*2	*ADC*1	*ADC*2	*ADC*1	*ADC*2
Acetaldehyde	–6.22	–6.10	–7.88	–8.00	–7.14	–6.09
Propanal	–6.24	–6.48	–7.89	–8.72	–7.11	–5.84
Butanal	–6.25	–6.94	–7.83	–7.99	–6.85	–7.67

Table S2 Calculated frequencies of the stationary points at the MPWB1K/6-311G(d,p) level.

Species	MPWB1K/6-311G(d, p)
*ADC*1-AH+NO_2→products	
CH_3CHO	163 (150), 517 (509), 790 (763), 919 (867), 1157 (919), 1165 (1113), 1401 (1352), 1461 (1400), 1487 (1420), 1497 (1441), 1919 (1743), 2968 (2822), 3106 (2917), 3178 (2967), 3231 (3005)
*ADC*1-AH	22, 60, 73, 103, 110, 157, 173, 223, 247, 287, 320, 370, 375, 392, 429, 533, 697, 807, 817, 826, 839, 854, 934, 960, 991, 1047,1067, 1172, 1183, 1408, 1482, 1496, 1519, 1886, 3041,3109, 3180, 3236, 3772, 4034, 4044, 4048
adsorbed-CH_3CO	27, 46,70, 105, 115, 131, 148, 217, 254, 288, 316, 365, 373, 387, 424, 496, 616, 808, 822, 836, 846, 899, 907, 973, 979, 1041, 1048, 1092, 1389, 1480, 1487, 2017, 3112, 3205, 3225, 3915, 4038, 4045, 4049
syn-TS_{CH3}	2000*i*, 20, 39, 48, 67, 78, 85, 104, 141, 153, 211, 248, 256, 280, 287, 353, 370, 387, 399, 476, 503, 515, 589, 632, 809, 822, 835, 846, 866, 928, 937, 988, 1007, 1037, 1049, 1118, 1148, 1193, 1268, 1413, 1464, 1513, 1735, 1812, 3108, 3176, 3285, 3859, 4031, 4044, 4048
n-TS_{CH3}	1623*i*, 14, 23, 27, 34, 66, 68, 89, 120, 156, 220, 245, 266, 289, 319, 330, 369, 378, 390, 430, 432, 514, 652, 697, 807, 826, 839, 855, 865, 946, 961, 984, 1021, 1047, 1061, 1139, 1170, 1268, 1458, 1508, 1511, 1542, 1748, 1843, 3087, 3189, 3302, 3815, 4034, 4043, 4046,
*ADC*2-AH+NO_2→products	
*ADC*2-AH	26, 47, 65, 114, 127, 160, 168, 222, 249, 290, 313, 368, 374, 394, 426, 551, 707, 797, 806, 826, 839, 847, 927, 954, 983, 1042, 1064, 1169, 1184, 1415, 1462, 1496, 1503, 1893, 3010, 3108, 3177, 3244, 3785, 4038, 4043, 4048
adsorbed-CH_3CO	24, 59, 77, 98, 118, 158, 223, 247, 286, 320, 369, 374, 392, 429, 473, 524, 700, 796, 807, 826, 839, 855, 958, 990, 1011, 1042, 1048, 1069, 1207, 1456, 1522, 1616, 3098, 3224, 3348, 3771, 4034, 4044, 4048
adsorbed-CH_2CHO	33, 51, 71, 124, 138, 171, 219, 255, 286, 316, 369, 374, 394, 427, 482, 544, 697, 807, 822, 825, 839, 854, 952, 980, 1013, 1017, 1043, 1067, 1217, 1436, 1531, 1611, 3080, 3217, 3340, 3767, 4035, 4043, 4049
syn-TS_{CHO}	1666*i*, 12, 19, 41, 60, 66, 81, 95, 133, 161, 177, 211, 261, 285, 292, 318, 362, 370, 372, 382, 389, 420, 569, 588, 807, 818, 829, 840, 868, 882, 939, 975, 1003, 1035, 1046, 1137, 1291, 1300, 1397, 1401, 1486, 1495, 1693, 1985, 3120, 3207, 3243, 3952, 4037, 4045, 4049
syn-TS_{CH3}	2065*i*, 66, 72, 91, 108, 116, 131, 141, 161, 175, 200, 237, 256, 295, 311, 329, 375, 386, 397, 439, 474, 523, 654, 735, 809, 829, 835, 846, 851, 932, 970, 993, 1008, 1042, 1082, 1104, 1158, 1232, 1262, 1418, 1443, 1491, 1767, 1805, 3052, 3191, 3297, 3806, 4036, 4041, 4043,
n-TS_{CHO}	1797*i*, 11, 20, 34, 50, 58, 77, 90, 124, 165, 195, 213, 259, 267, 286, 293, 316, 362, 372, 382, 419, 424, 533, 568, 807,

	817, 830, 842, 857, 884, 923, 975, 988, 1037, 1047, 1127, 1293, 1401, 1477, 1491, 1504, 1606, 1807, 2000, 3113, 3201, 3236, 3955, 4037, 4046, 4049
n-TS_{CH3}	1934*i*, 55, 62, 78, 119, 122, 143, 148, 194, 200, 219, 231, 256, 306, 351, 372, 387, 406, 413, 429, 522, 536, 636, 754, 810, 824, 846, 869, 911, 924, 957, 972, 1028, 1045, 1060, 1122, 1171, 1328, 1444, 1503, 1509, 1561, 1775, 1833, 3057, 3180, 3292, 3797, 3993, 4043, 4046
*ADC*1-PN+NO_2→products	
CH_3CH_2CHO	119 (135), 232 (220), 251 (271), 680 (660), 690 (668), 895 (848), 921 (892), 1023 (993), 1141 (1093), 1173 (1118), 1304 (1250), 1400 (1335), 1437 (1376), 1449 (1390), 1478 (1416), 1515 (1451), 1526 (1460), 1910 (1743), 2974 (2809), 3094 (2895), 3124 (2904), 3126 (2941), 3205 (2981), 3206 (2992)
*ADC*1-PN	18, 28, 62, 75, 88, 130, 137, 222, 242, 248, 281, 292, 323, 370, 375, 393, 430, 680, 692, 710, 806, 826, 839, 855, 909, 938, 959, 993, 1027, 1048, 1067, 1144, 1184, 1307, 1406, 1442, 1468, 1506, 1515, 1528, 1876, 3040, 3097, 3125, 3127, 3206, 3209, 3775, 4035, 4043, 4048
adsorbed-CH_2CH_2CHO	24, 36, 67, 79, 93, 135, 167, 196, 223, 248, 287, 324, 332, 370, 376, 393, 430, 448, 680, 696, 716, 807, 825, 838, 857, 916, 957, 992, 1022, 1044, 1047, 1066, 1157, 1238, 1406, 1437, 1479, 1513, 1880, 3037, 3055, 3057, 3238, 3357, 3788, 4034, 4044, 4048
adsorbed-CH_3CHCHO	34, 47, 61, 84, 105, 119, 142, 218, 243, 285, 316, 328, 354, 368, 379, 394, 431, 682, 714, 737, 809, 834, 846, 849, 927, 971, 987, 997, 1053, 1055, 1085, 1096, 1208, 1407, 1444, 1466, 1499, 1533, 1638, 3088, 3106, 3140, 3224, 3253, 3749, 4041, 4042, 4048
syn-TS_{CH3}	1851*i*, 26, 30, 35, 53, 58, 80, 95, 126, 165, 201, 213, 247, 261, 271, 281, 322, 338, 366, 382, 392, 431, 490, 555, 664, 715, 731, 807, 829, 844, 846, 858, 909, 964, 976, 987, 1027, 1044, 1066, 1146, 1166, 1226, 1243, 1284, 1408, 1448, 1453, 1472, 1493, 1741, 1876, 3059, 3073, 3159, 3172, 3268, 3814, 4040, 4040, 4043
n-TS_{CH3}	1370*i*, 19, 25, 44, 55, 72, 90, 114, 144, 165, 204, 217, 257, 274, 279, 297, 315, 321, 368, 369, 391, 423, 479, 588, 654, 699, 729, 806, 819, 833, 855, 863, 915, 952, 969, 987, 1018, 1044, 1060, 1152, 1164, 1264, 1293, 1404, 1459, 1476, 1505, 1516, 1620, 1819, 1874, 3052, 3071, 3133, 3188, 3292, 3838, 4033, 4047, 4051
syn-TS_{CH2}	2026*i*, 23, 25, 34, 56, 58, 78, 107, 118, 139, 156, 201, 216, 247, 281, 285, 299, 320, 336, 368, 379, 392, 432, 513, 665, 704, 787, 809, 829, 843, 849, 892, 936, 968, 985, 993, 1047, 1068, 1085, 1133, 1160, 1214, 1255, 1382, 1411, 1446, 1488, 1510, 1517, 1742, 1810, 3071, 3102, 3181, 3207, 3225, 3802, 4040, 4041, 4044
n-TS_{CH2}	1832*i*, 11, 19, 29, 34, 57, 61, 85, 115, 130, 182, 219, 231, 241, 267, 286, 307, 327, 345, 370, 376, 389, 430, 494, 649, 715, 805, 823, 838, 854, 856, 867, 931, 952, 984, 1005, 1045, 1061, 1083, 1148, 1183, 1291, 1406, 1440, 1481, 1503, 1509, 1519, 1532, 1772, 1833, 3081, 3098, 3171, 3199, 3222, 3805, 4033, 4042, 4046
*ADC*2-PN+NO_2→products	

*ADC*2-PN	41, 58, 92, 106, 117, 142, 218, 221, 240, 277, 292, 311, 358, 364, 375, 396, 430, 676, 698, 712, 808, 836, 846, 851, 897, 932, 972, 976, 1028, 1031, 1069, 1154, 1200, 1325, 1408, 1449, 1458, 1480, 1538, 1567, 1894, 3008, 3093, 3123, 3134, 3213, 3231, 3831, 4041, 4044, 4046
adsorbed-CH_3CH_2CO	42, 58, 90, 103, 122, 129, 199, 218, 239, 270, 292, 311, 362, 373, 385, 390, 428, 586, 654, 786, 808, 833, 842, 846, 861, 894, 977, 1011, 1030, 1059, 1111, 1129, 1320, 1349, 1454, 1469, 1535, 1573, 2014, 3126, 3131, 3162, 3210, 3238, 3910, 4041, 4044, 4046
adsorbed-CH_2CH_2CHO	30, 47, 73, 85, 117, 136, 187, 218, 242, 268, 279, 291, 314, 362, 375, 393, 431, 587, 636, 686, 759, 805, 838, 846, 853, 885, 902, 943, 973, 1020, 1068, 1120, 1168, 1298, 1348, 1440, 1463, 1536, 1893, 3003, 3069, 3123, 3236, 3352, 3821, 4040, 4041, 4044
adsorbed-CH_3CHCHO	31, 46, 76, 102, 121, 150, 216, 241, 270, 286, 294, 319, 350, 366, 375, 398, 432, 647, 684, 723, 806, 835, 846, 851, 944, 951, 974, 979, 1030, 1046, 1072, 1100, 1194, 1422, 1443, 1476, 1518, 1538, 1648, 3074, 3090, 3165, 3214, 3252, 3762, 4040, 4042, 4044,
syn-TS_{CHO}	1683*i*, 19, 27, 51, 54, 71, 80, 98, 120, 136, 151, 220, 241, 258, 289, 307, 321, 326, 365, 372, 374, 390, 399, 429, 538, 703, 766, 808, 832, 841, 846, 863, 867, 933, 978, 1027, 1030, 1054, 1086, 1132, 1277, 1288, 1320, 1371, 1400, 1451, 1471, 1533, 1557, 1694, 1981, 3121, 3128, 3161, 3210, 3223, 3950, 4041, 4042, 4044
syn-TS_{CH3}	1787*i*, 31, 45, 60, 63, 70, 84, 111, 116, 148, 170, 198, 214, 230, 243, 246, 301, 321, 352, 371, 386, 430, 534, 588, 625, 695, 718, 805, 823, 832, 842, 861, 878, 915, 933, 978, 1033, 1047, 1103, 1126, 1166, 1204, 1232, 1307, 1366, 1419, 1441, 1474, 1520, 1750, 1891, 3017, 3101, 3141, 3196, 3292, 3892, 4003, 4042, 4048
syn-TS_{CH2}	2034*i*, 23, 32, 42, 64, 82, 86, 101, 127, 140, 157, 218, 242, 265, 274, 281, 298, 310, 325, 365, 376, 391, 429, 512, 683, 714, 775, 807, 832, 840, 847, 893, 930, 950, 974, 987, 1034, 1066, 1086, 1135, 1163, 1216, 1252, 1373, 1413, 1443, 1455, 1512, 1524, 1745, 1826, 3046, 3107, 3187, 3197, 3225, 3850, 4040, 4043, 4046
n-TS_{CHO}	1794*i*, 16, 19, 40, 46, 56, 87, 99, 107, 147, 204, 217, 228, 239, 280, 287, 291, 309, 319, 362, 374, 385, 421, 429, 563, 691, 775, 808, 829, 840, 843, 848, 884, 917, 975, 1020, 1031, 1053, 1089, 1129, 1272, 1321, 1378, 1449, 1464, 1497, 1527, 1553, 1608, 1805, 1997, 3119, 3131, 3154, 3215, 3225, 3949, 4041, 4043, 4046
n-TS_{CH3}	1226*i*, 15, 27, 42, 57, 63, 89, 104, 124, 143, 203, 214, 223, 227, 256, 293, 319, 323, 369, 375, 395, 431, 517, 618, 650, 694, 726, 809, 831, 840, 849, 866, 915, 931, 946, 976, 1030, 1065, 1119, 1135, 1173, 1292, 1326, 1386, 1443, 1470, 1513, 1516, 1602, 1815, 1891, 3020, 3099, 3138, 3189, 3292, 3832, 4039, 4041, 4045
n-TS_{CH2}	-1872*i*, 24, 26, 50, 58, 68, 79, 118, 142, 154, 201, 219, 246, 259, 279, 286, 320, 328, 337, 363, 379, 390, 430, 487, 609, 709, 806, 833, 837, 842, 859, 867, 920, 926, 975, 992, 1025, 1060, 1083, 1134, 1182, 1288, 1407, 1448, 1453, 1503, 1516, 1525, 1540, 1791, 1831, 3064, 3107, 3177, 3199, 3215, 3847, 4036, 4041, 4046
*ADC*1-BN+NO_2→products	

$CH_3CH_2CH_2CHO$	88, 186, 200, 240, 347, 678, 717, 800, 889, 969, 987, 1096, 1168, 1181, 1275, 1341, 1358, 1433, 1444, 1449, 1477, 1516, 1525, 1534, 1908, 2969, 3082, 3099, 3113, 3127, 3156, 3181, 3185
*ADC*1-BN	17, 32, 59, 62, 84, 98, 123, 209, 218, 235, 251, 257, 286, 322, 357, 371, 375, 393, 430, 681, 696, 735, 806, 811, 825, 838, 854, 899, 958, 982, 987, 1004, 1047, 1068, 1097, 1169, 1190, 1279, 1342, 1355, 1436, 1449, 1469, 1512, 1519, 1529, 1535, 1874, 3040, 3085, 3101, 3114, 3127, 3158, 3182, 3188, 3770, 4035, 4044, 4048
adsorbed-$CH_2CH_2CH_2CHO$	15, 31, 61, 62, 67, 85, 108, 124, 211, 220, 239, 252, 286, 322, 343, 370, 374, 392, 430, 509, 677, 692, 732, 804, 806, 825, 838, 853, 936, 957, 972, 992, 1046, 1064, 1082, 1123, 1177, 1272, 1316, 1354, 1415, 1462, 1492, 1509, 1518, 1874, 3039, 3097, 3118, 3128, 3166, 3212, 3321, 3780, 4035, 4043, 4047
adsorbed-CH_3CHCH_2CHO	21, 32, 47, 59, 66, 83, 97, 122, 190, 219, 235, 251, 287, 320, 325, 366, 373, 376, 393, 430, 680, 718, 732, 807, 825, 838, 856, 898, 957, 985, 991, 1002, 1047, 1054, 1067, 1148, 1189, 1240, 1315, 1428, 1441, 1470, 1500, 1508, 1516, 1878, 3019, 3040, 3045, 3051, 3094, 3193, 3284, 3778, 4034, 4044, 4048
adsorbed-CH_3CH_2CHCHO	26, 35, 53, 64, 83, 101, 137, 216, 228, 243, 262, 284, 329, 330, 366, 379, 395, 417, 431, 690, 715, 753, 808, 810, 834, 847, 851, 910, 970, 993, 1022, 1051, 1056, 1082, 1088, 1111, 1220, 1299, 1350, 1434, 1457, 1496, 1515, 1527, 1535, 1637, 3075, 3093, 3111, 3177, 3196, 3200, 3241, 3745, 4040, 4043, 4046
syn-TS_{CH3}	1806*i*, 16, 24, 29, 44, 52, 61, 91, 101, 112, 123, 160, 210, 223, 248, 259, 282, 301 315, 328, 366, 378, 390, 430, 543, 558, 660, 697, 729, 806, 817, 831, 844, 847, 880, 924, 965, 980, 997, 1023, 1045, 1065, 1106, 1123, 1192, 1201, 1247, 1286, 1334, 1357, 1423, 1432, 1465, 1486, 1492, 1521, 1746, 1881, 3037, 3097, 3131, 3138, 3153, 3186, 3248, 3792, 4039, 4041, 4044,
n-TS_{CH3}	1359*i*, 14, 17, 20, 32, 41, 67, 86, 87, 98, 118, 190, 214, 222, 235, 252, 290, 292, 329, 370, 376, 378, 393, 431, 465, 593, 667, 684, 733, 806, 825, 826, 839, 855, 862, 898, 953, 980, 993, 1002, 1043, 1063, 1132, 1168, 1173, 1243, 1301, 1319, 1351, 1442, 1469, 1485, 1488, 1506, 1515, 1577, 1812, 1875, 3055, 3071, 3096, 3136, 3150, 3163, 3259, 3799, 4034, 4043, 4047
syn-$TS_{CH2}1$	1828*i*, 13, 15, 29, 43, 59, 74, 81, 102, 120, 140, 152, 196, 221, 228, 249, 265, 288, 292, 322, 367, 372, 374, 391, 428, 511, 649, 709, 731, 806, 822, 832, 836, 856, 892, 904, 952, 981, 1001, 1006, 1045, 1060, 1125, 1163, 1183, 1209, 1231, 1279, 1333, 1420, 1430, 1444, 1467, 1507, 1514, 1520, 1744, 1880, 3049, 3063, 3082, 3119, 3157, 3202, 3213, 3818, 4034, 4042, 4049
n-$TS_{CH2}1$	1539*i*, 20, 27, 37, 51, 61, 79, 102, 122, 131, 164, 184, 199, 207, 233, 237, 286, 296, 320, 348, 366, 387, 396, 413, 428, 464, 677, 714, 734, 807, 835, 842, 848, 872, 874, 901, 963, 976, 992, 1006, 1041, 1075, 1142, 1167, 1183, 1263, 1319, 1334, 1427, 1446, 1468, 1484, 1509, 1512, 1518, 1603, 1812, 1865, 3047, 3073, 3091, 3121, 3150, 3192, 3208, 3783, 4034, 4042, 4048
syn-$TS_{CH2}2$	1964*i*, 18, 37, 41, 55, 81, 91, 102, 110, 121, 141, 159, 225, 230, 239, 260, 282, 303, 331, 360, 366, 369, 388, 408, 470, 515, 641, 724, 761, 807, 831, 846, 850, 865, 875, 906, 965, 983, 1025, 1049, 1051, 1063, 1108, 1160, 1185, 1217,

	1276, 1295, 1327, 1389, 1448, 1456, 1492, 1501, 1530, 1535, 1728, 1820, 3074, 3093, 3110, 3157, 3183, 3189, 3199, 3819, 4033, 4043, 4045
n-TS_{CH2}2	-1848*i*, 15, 21, 23, 36, 45, 68, 78, 87, 112, 128, 181, 213, 225, 243, 257, 270, 288, 327, 343, 361, 371, 379, 391, 432, 493, 661, 730, 768, 805, 826, 839, 858, 862, 882, 916, 955, 984, 1023, 1046, 1052, 1063, 1106, 1156, 1189, 1288, 1291, 1331, 1442, 1450, 1482, 1493, 1503, 1526, 1531, 1536, 1774, 1831, 3078, 3084, 3112, 3153, 3187, 3191, 3203, 3808, 4033, 4042, 4047,
*ADC*2-BN+NO_2→products	
*ADC*2-BN	32, 57, 65, 81, 94, 129, 148, 206, 215, 230, 246, 269, 291, 314, 353, 361, 376, 394, 430, 617, 696, 720, 806, 827, 835, 846, 850, 897, 919, 971, 980, 995, 1028, 1064, 1104, 1171, 1191, 1282, 1346, 1374, 1436, 1445, 1454, 1474, 1521, 1533, 1538, 1889, 3005, 3083, 3101, 3112, 3133, 3161, 3190, 3204, 3822, 4041, 4042, 4045,
adsorbed-$CH_3CH_2CH_2CO$	39, 62, 78, 84, 102, 117, 156, 194, 199, 221, 247, 265, 292, 316, 347, 361, 375, 390, 429, 598, 671, 759, 807, 831, 844, 849, 854, 885, 898, 961, 974, 1032, 1055, 1096, 1104, 1151, 1267, 1308, 1359, 1405, 1441, 1466, 1526, 1532, 1559, 2010, 3102, 3114, 3131, 3148, 3164, 3189, 3202, 3910, 4040, 4041, 4045
adsorbed-$CH_2CH_2CH_2CHO$	37, 49, 81, 86, 95, 132, 134, 191, 215, 224, 229, 252, 294, 309, 363, 368, 376, 394, 427, 493, 628, 698, 724, 806, 835, 845, 849, 862, 908, 931, 972, 981, 1030, 1063, 1082, 1142, 1167, 1232, 1334, 1357, 1446, 1449, 1473, 1487, 1531, 1890, 3009, 3058, 3088, 3114, 3131, 3216, 3335, 3825, 4041, 4043, 4045
adsorbed-CH_3CH_2CHCHO	44, 52, 70, 96, 100, 146, 175, 223, 227, 249, 264, 297, 315, 352, 365, 373, 378, 398, 433, 633, 673, 746, 805, 825, 835, 847, 854, 930, 941, 970, 999, 1029, 1067, 1087, 1119, 1126, 1200, 1326, 1376, 1442, 1444, 1509, 1517, 1536, 1537, 1652, 3069, 3071, 3108, 3127, 3181, 3206, 3239, 3745, 4039, 4040, 4043
syn-TS_{CHO}	1671*i*, 18, 31, 52, 56, 66, 74, 81, 102, 112, 143, 158, 211, 221, 245, 269, 290, 292, 316, 355, 361, 370, 374, 385, 393, 427, 558, 729, 763, 808, 827, 840, 849, 851, 885, 892, 921, 974, 992, 1032, 1052, 1098, 1108, 1157, 1260, 1290, 1307, 1328, 1362, 1397, 1421, 1447, 1469, 1528, 1532, 1553, 1693, 1977, 3104, 3110, 3133, 3151, 3168, 3194, 3202, 3947, 4040, 4042, 4046,
n-TS_{CHO}	1804*i*, 10, 23, 39, 44, 65, 79, 89, 98, 101, 172, 176, 218, 228, 247, 261, 266, 287, 294, 319, 354, 363, 372, 387, 420, 428, 564, 718, 778, 807, 828, 840, 849, 860, 864, 888, 900, 975, 981, 1032, 1052, 1101, 1112, 1155, 1260, 1309, 1333, 1383, 1419, 1437, 1462, 1497, 1522, 1531, 1572, 1604, 1805, 1993, 3105, 3108, 3136, 3144, 3168, 3192, 3207, 3946, 4039, 4041, 4045,
syn-TS_{CH3}	1744*i*, 16, 27, 42, 56, 65, 88, 101, 111, 131, 152, 207, 224, 231, 241, 253, 263, 297, 319, 366, 373, 381, 395, 431, 525, 581, 681, 703, 724, 806, 828, 830, 842, 857, 881, 918, 947, 971, 992, 1007, 1036, 1063, 1135, 1149, 1182, 1211, 1241, 1257, 1329, 1370, 1421, 1446, 1449, 1477, 1496, 1537, 1754, 1890, 3020, 3082, 3092, 3125, 3160, 3177, 3279, 3830, 4037, 4042, 4044

n-TS_{CH3}	1230*i*, 20, 30, 36, 59, 72, 99, 117, 128, 135, 169, 207, 224, 235, 249, 258, 296, 309, 326, 367, 375, 383, 396, 434, 495, 600, 628, 710, 726, 804, 831, 845, 861, 864, 872, 905, 919, 966, 994, 1004, 1030, 1064, 1145, 1173, 1187, 1253, 1300, 1337, 1366, 1447, 1449, 1474, 1488, 1514, 1538, 1582, 1807, 1888, 3023, 3079, 3095, 3130, 3149, 3170, 3278, 3829, 4034, 4040, 4044
syn-TS_{CH2}	1973*i*, 18, 30, 37, 63, 80, 90, 95, 126, 139, 152, 199, 222, 233, 248, 253, 273, 295, 311, 330, 365, 371, 380, 394, 428, 512, 656, 724, 798, 806, 827, 841, 852, 861, 869, 916, 926, 969, 1000, 1032, 1058, 1070, 1116, 1155, 1188, 1209, 1274, 1310, 1343, 1382, 1442, 1453, 1458, 1526, 1537, 1542, 1732, 1831, 3071, 3085, 3110, 3146, 3175, 3182, 3219, 3841, 4040, 4041, 4046
n-TS_{CH2}	1882*i*, 16, 21, 24, 69, 73, 80, 97, 117, 131, 149, 196, 219, 228, 247, 257, 267, 297, 316, 340, 358, 368, 376, 393, 431, 498, 646, 727, 803, 808, 830, 844, 851, 857, 874, 922, 934, 971, 1012, 1031, 1058, 1069, 1112, 1160, 1183, 1282, 1303, 1344, 1437, 1446, 1455, 1501, 1515, 1521, 1533, 1539, 1792, 1831, 3058, 3088, 3109, 3142, 3182, 3188, 3205, 3831, 4039, 4041, 4044

The values in parentheses are the available published data [1].

Table S3 The rate constants (cm^3 $molecule^{-1}$ s^{-1}) of each channel involve in the reaction of NO_2 with adsorbed acetaldehyde at different temperatures and altitudes in the Earth atmosphere.

		ADC1-AH		*ADC2*-AH				
h (km)	*T* (K)	*syn*-R_{CH3}	*n*-R_{CH3}	*syn*-R_{CHO}	*syn*-R_{CH3}	*n*-R_{CHO}	*n*-R_{CH3}	k_{total}(AH)
0	298.15	1.79×10^{-34}	1.37×10^{-35}	8.00×10^{-25}	4.18×10^{-34}	2.79×10^{-29}	6.97×10^{-34}	8.00×10^{-25}
0	288.19	4.29×10^{-35}	2.43×10^{-36}	3.09×10^{-25}	1.14×10^{-34}	7.64×10^{-30}	1.54×10^{-34}	3.09×10^{-25}
2	275.21	5.91×10^{-36}	2.13×10^{-37}	8.17×10^{-26}	1.86×10^{-35}	1.23×10^{-30}	1.85×10^{-35}	8.17×10^{-26}
4	262.23	7.02×10^{-37}	1.49×10^{-38}	1.93×10^{-26}	2.66×10^{-36}	1.68×10^{-31}	1.82×10^{-36}	1.93×10^{-26}
6	249.25	7.15×10^{-38}	8.02×10^{-40}	4.01×10^{-27}	3.24×10^{-37}	1.87×10^{-32}	1.42×10^{-37}	4.01×10^{-27}
8	236.27	6.18×10^{-39}	3.19×10^{-41}	7.17×10^{-28}	3.31×10^{-38}	1.65×10^{-33}	8.47×10^{-39}	7.17×10^{-28}
10	223.29	4.48×10^{-40}	8.92×10^{-43}	1.07×10^{-28}	2.77×10^{-39}	1.11×10^{-34}	3.69×10^{-40}	1.07×10^{-28}
12	216.69	1.09×10^{-40}	1.24×10^{-43}	3.78×10^{-29}	7.19×10^{-40}	2.48×10^{-35}	6.53×10^{-41}	3.78×10^{-29}

Table S4 The rate constants (cm^3 $molecule^{-1}$ s^{-1}) of each channel involve in the reaction of NO_2 with adsorbed propanal at different temperatures and altitudes in the Earth atmosphere.

		ADC1-PN					
h (km)	*T* (K)	*syn*-R_{CH3}	*syn*-R_{CH2}	*n*-R_{CH3}	*n*-R_{CH2}	k_{total}(PN)	
0	298.15	9.40×10^{-34}	5.08×10^{-30}	6.47×10^{-37}	1.55×10^{-31}	2.22×10^{-24}	
0	288.19	2.04×10^{-34}	1.71×10^{-30}	1.04×10^{-37}	4.61×10^{-32}	8.70×10^{-25}	
2	275.21	2.39×10^{-35}	3.82×10^{-31}	7.84×10^{-39}	8.45×10^{-33}	2.34×10^{-25}	
4	262.23	2.29×10^{-36}	7.74×10^{-32}	4.63×10^{-40}	1.33×10^{-33}	5.65×10^{-26}	
6	249.25	1.75×10^{-37}	1.41×10^{-32}	2.05×10^{-41}	1.75×10^{-34}	1.20×10^{-26}	
8	236.27	1.02×10^{-38}	2.33×10^{-33}	6.50×10^{-43}	1.87×10^{-35}	2.19×10^{-27}	
10	223.29	4.34×10^{-40}	3.43×10^{-34}	1.39×10-44	1.57×10^{-36}	3.35×10^{-28}	
12	216.69	7.60×10^{-41}	1.24×10^{-34}	1.65×10-45	3.99×10^{-37}	1.20×10^{-28}	
		ADC2-PN					
[a] *h* (km)	*T* (K)	*syn*-R_{CHO}	*syn*-R_{CH3}	*syn*-R_{CH2}	*n*-R_{CHO}	*n*-R_{CH3}	*n*-R_{CH2}
0	298.15	2.22×10^{-24}	1.33×10^{-34}	4.45×10^{-30}	5.41×10^{-29}	2.24×10^{-37}	7.40×10^{-31}
0	288.19	8.70×10^{-25}	2.67×10^{-35}	1.41×10^{-30}	1.53×10^{-29}	3.79×10^{-38}	1.93×10^{-31}
2	275.21	2.34×10^{-25}	2.79×10^{-36}	2.86×10^{-31}	2.61×10^{-30}	3.12×10^{-39}	2.93×10^{-32}
4	262.23	5.65×10^{-26}	2.36×10^{-37}	5.14×10^{-32}	3.76×10^{-31}	2.01×10^{-40}	3.78×10^{-33}
6	249.25	1.20×10^{-26}	1.57×10^{-38}	8.09×10^{-33}	4.46×10^{-32}	9.82×10^{-42}	4.03×10^{-34}
8	236.27	2.19×10^{-27}	7.89×10^{-40}	1.10×10^{-33}	4.23×10^{-33}	3.46×10^{-43}	3.47×10^{-35}
10	223.29	3.35×10^{-28}	2.91×10^{-41}	1.29×10^{-34}	3.08×10^{-34}	8.32×10^{-45}	2.34×10^{-36}
12	216.69	1.20×10^{-28}	4.65×10^{-42}	4.08×10^{-35}	7.25×10^{-35}	1.06×10^{-45}	5.34×10^{-37}

Table S5 The rate constants (cm^3 $molecule^{-1}$ s^{-1}) of each channel involve in the reaction of NO_2 with adsorbed butanal at different temperatures and altitudes in the Earth atmosphere.

		ADC1-BN						
h (km)	*T* (K)	*syn*-R_{CH3}	*syn*-R_{CH2}1	*syn*-R_{CH2}2	*n*-R_{CH3}	*n*-R_{CH2}1	*n*-R_{CH2}2	k_{total}(BN)
0	298.15	1.50×10^{-32}	1.82×10^{-31}	8.18×10^{-30}	1.20×10^{-35}	8.75×10^{-33}	7.73×10^{-31}	2.80×10^{-24}
0	288.19	3.20×10^{-33}	4.74×10^{-32}	2.74×10^{-30}	2.05×10^{-36}	1.92×10^{-33}	1.97×10^{-31}	1.08×10^{-25}
2	275.21	3.65×10^{-34}	7.19×10^{-33}	6.01×10^{-31}	1.71×10^{-37}	2.26×10-34	2.9×10^{-32}	2.88×10^{-25}
4	262.23	3.40×10^{-35}	9.23×10^{-34}	1.18×10^{-31}	1.12×10^{-38}	2.17×10^{-35}	3.61×10^{-33}	6.81×10^{-26}
6	249.25	2.51×10^{-36}	9.76×10^{-35}	2.02×10^{-32}	5.60×10^{-40}	1.64×10^{-36}	3.72×10^{-34}	1.41×10^{-26}
8	236.27	1.41×10^{-37}	8.25×10^{-36}	3.01×10^{-33}	2.02×10^{-41}	9.45×10^{-38}	4.00×10^{-35}	2.52×10^{-27}
10	223.29	5.78×10^{-39}	5.38×10^{-37}	3.85×10^{-34}	5.01×10^{-43}	4.25×10^{-39}	2.58×10^{-36}	3.76×10^{-28}
12	216.69	9.90×10^{-40}	1.19×10^{-37}	1.27×10^{-34}	6.47×10^{-44}	7.31×10^{-40}	5.73×10^{-37}	1.32×10^{-28}
		ADC2-BN						
[a] *h* (km)	*T* (K)	*syn*-R_{CHO}	*syn*-R_{CH3}	*syn*-R_{CH2}	*n*-R_{CHO}	*n*-R_{CH3}	*n*-R_{CH2}	
0	298.15	2.80×10^{-24}	5.66×10^{-32}	6.17×10^{-30}	3.98×10^{-27}	1.44×10^{-35}	3.65×10^{-31}	
0	288.19	1.08×10^{-25}	1.24×10^{-32}	1.99×10^{-30}	1.25×10^{-27}	2.56×10^{-36}	9.29×10^{-32}	
2	275.21	2.88×10^{-25}	1.51×10^{-33}	4.16×10^{-31}	2.45×10^{-28}	2.24×10^{-37}	1.37×10^{-32}	
4	262.23	6.81×10^{-26}	1.46×10^{-34}	7.69×10^{-32}	4.14×10^{-29}	1.56×10^{-38}	1.70×10^{-33}	
6	249.25	1.41×10^{-26}	1.12×10^{-35}	1.24×10^{-32}	5.84×10^{-30}	8.25×10^{-40}	1.74×10^{-34}	
8	236.27	2.52×10^{-27}	6.58×10^{-37}	1.74×10^{-33}	6.71×10^{-31}	3.18×10^{-41}	1.43×10^{-35}	
10	223.29	3.76×10^{-28}	2.83×10^{-38}	2.08×10^{-34}	6.07×10^{-32}	8.48×10^{-43}	9.11×10^{-37}	
12	216.69	1.32×10^{-28}	4.98×10^{-39}	6.64×10^{-35}	1.61×10^{-32}	1.14×10^{-43}	2.01×10^{-37}	

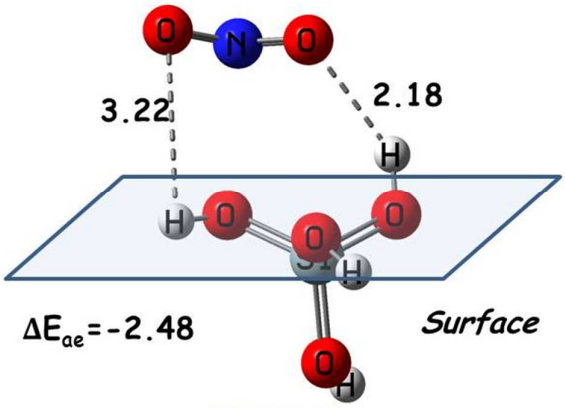


Fig. S1. The geometry of *ADC*1-NO_2 (in Å) as well as the corresponding adsorption energy (E_{ae}, in kcal mol^{-1}) from the reference [2].

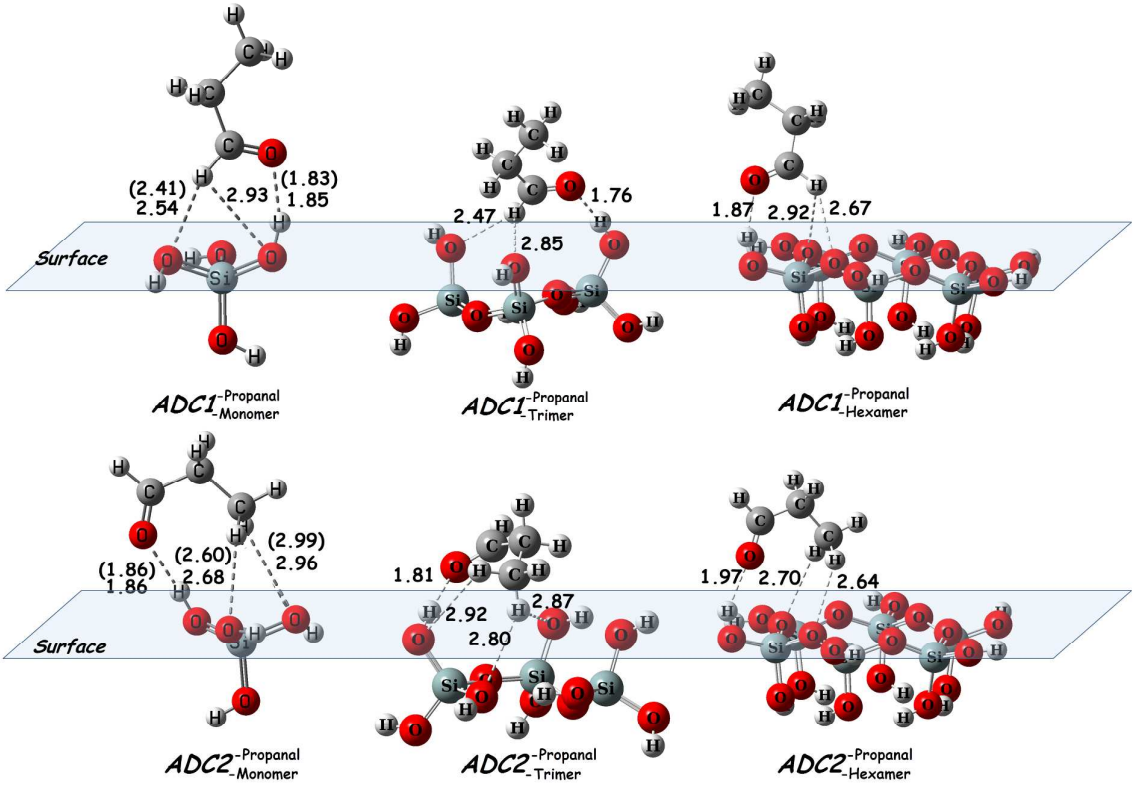


Fig. S2. The geometries of adsorption complexes for propanal onto three surface models (in Å).

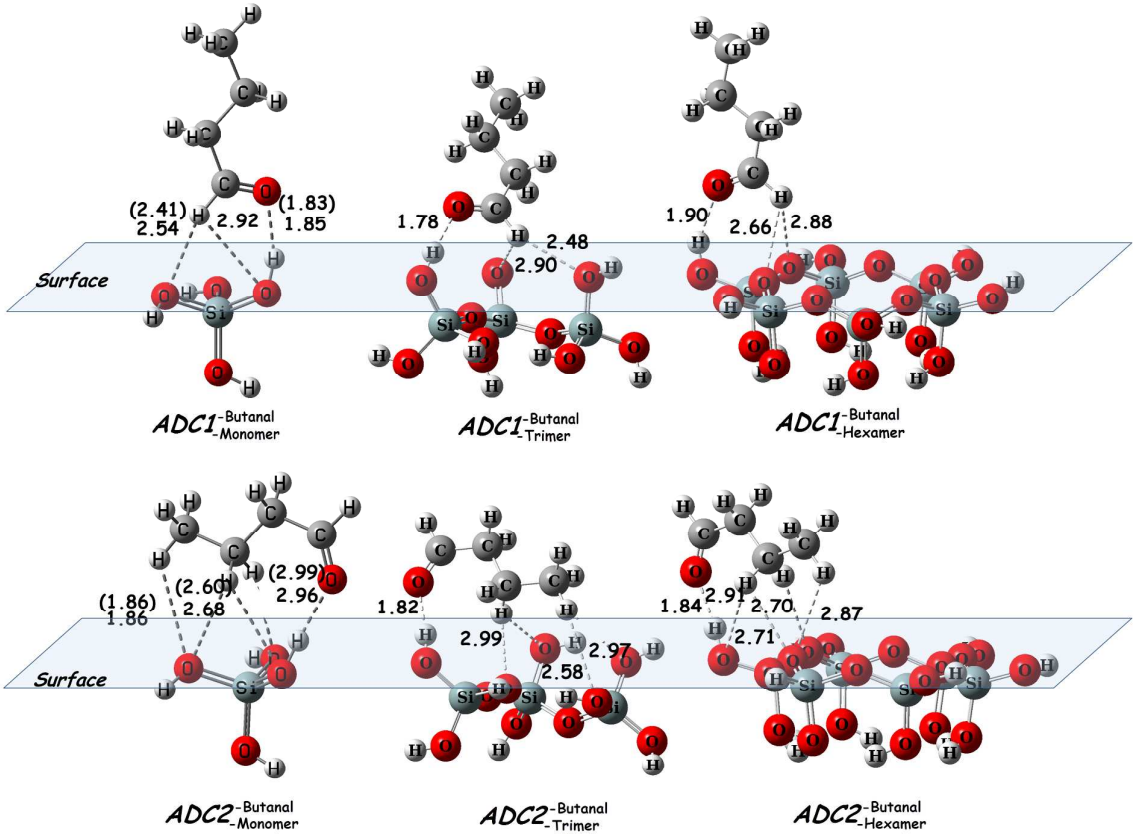


Fig. S3. The geometries of adsorption complexes for propanal onto three surface models (in Å).

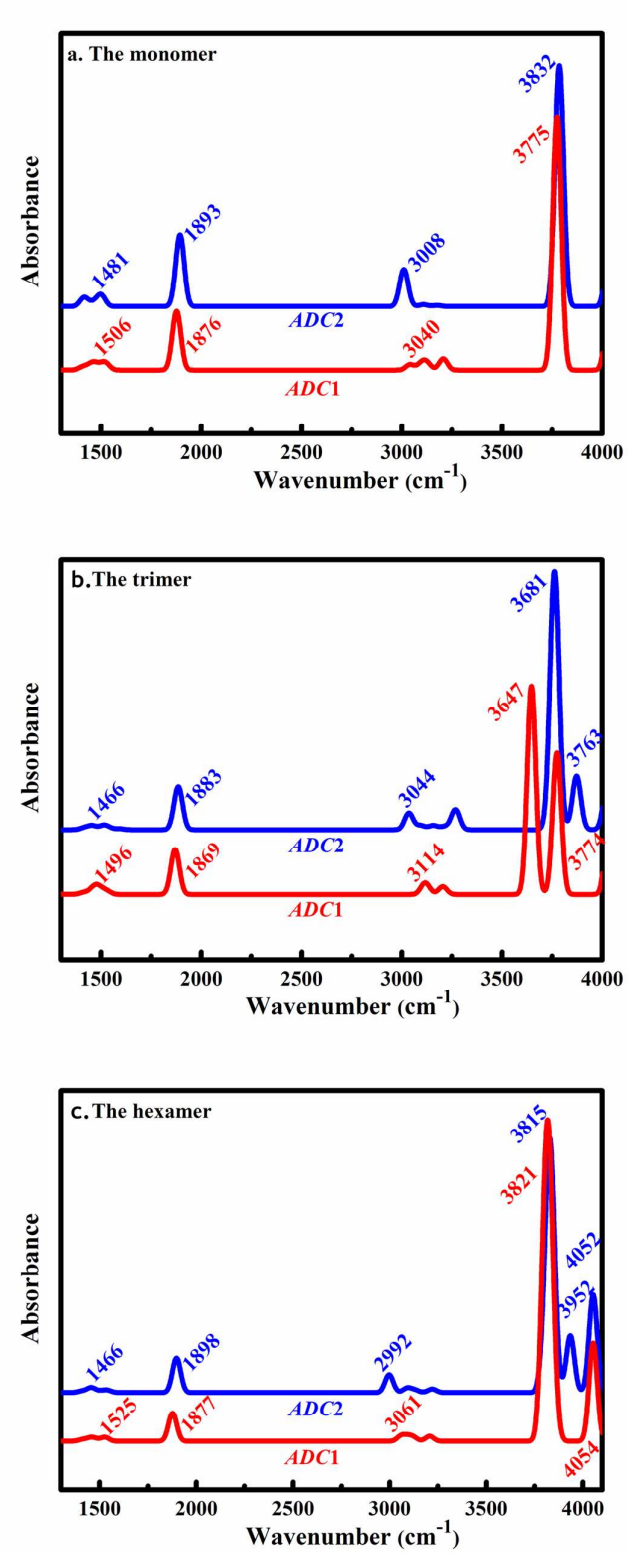


Fig. S4. The calculated infrared spectrum for the complexes of propanal adsorbed onto three surface models. The infrared data are cut off at 1300 cm^{-1}, because of intense lattice absorptions.

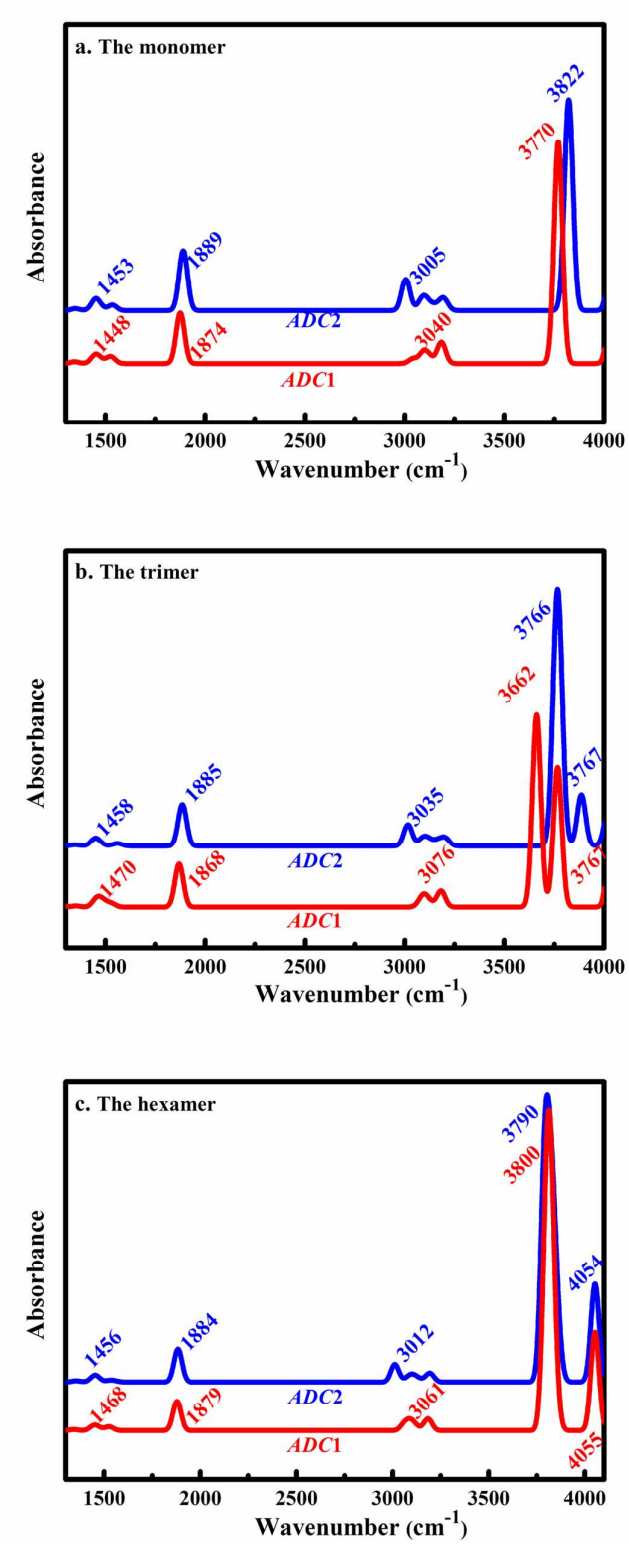
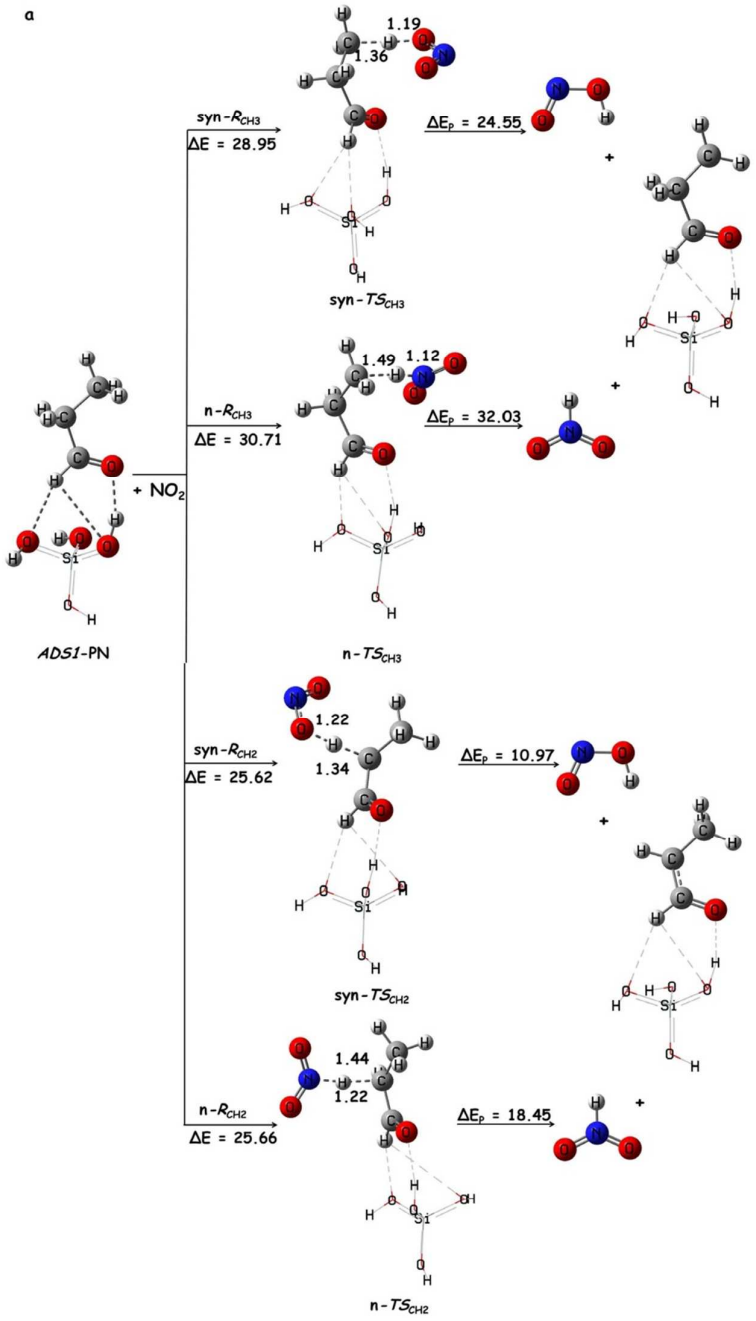


Fig. S5. The calculated infrared spectrum for the complexes of butanal adsorbed onto three surface models. The infrared data are cut off at 1300 cm^{-1}, because of intense lattice absorptions.


a
1.19
1.36
syn-R_{CH3}
ΔE = 28.95
ΔE$_P$ = 24.55
syn-TS_{CH3}
1.49
1.12
n-R_{CH3}
ΔE = 30.71
ΔE$_P$ = 32.03
+ NO_2
ADS1-PN
n-TS_{CH3}
1.22
1.34
syn-R_{CH2}
ΔE = 25.62
ΔE$_P$ = 10.97
syn-TS_{CH2}
1.44
1.22
n-R_{CH2}
ΔE = 25.66
ΔE$_P$ = 18.45
n-TS_{CH2}

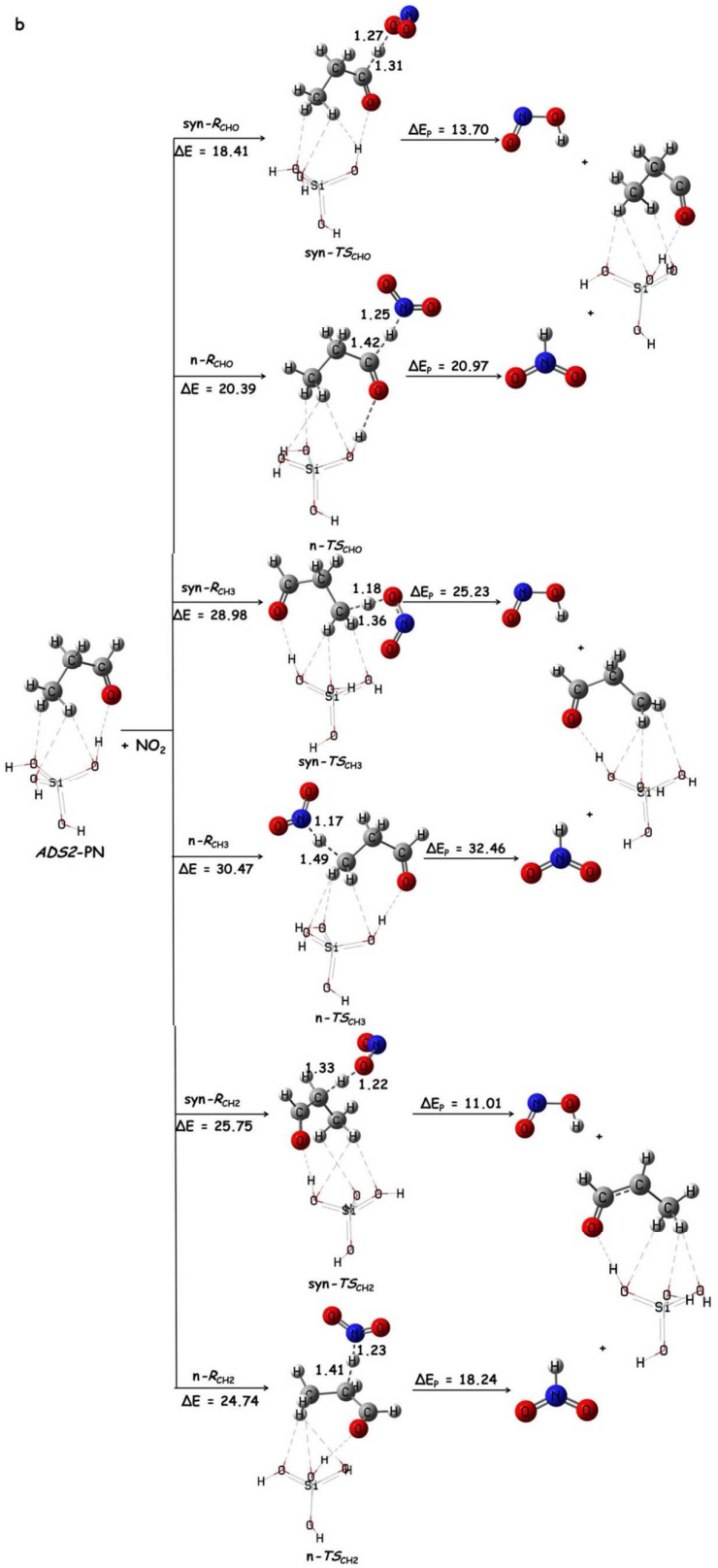
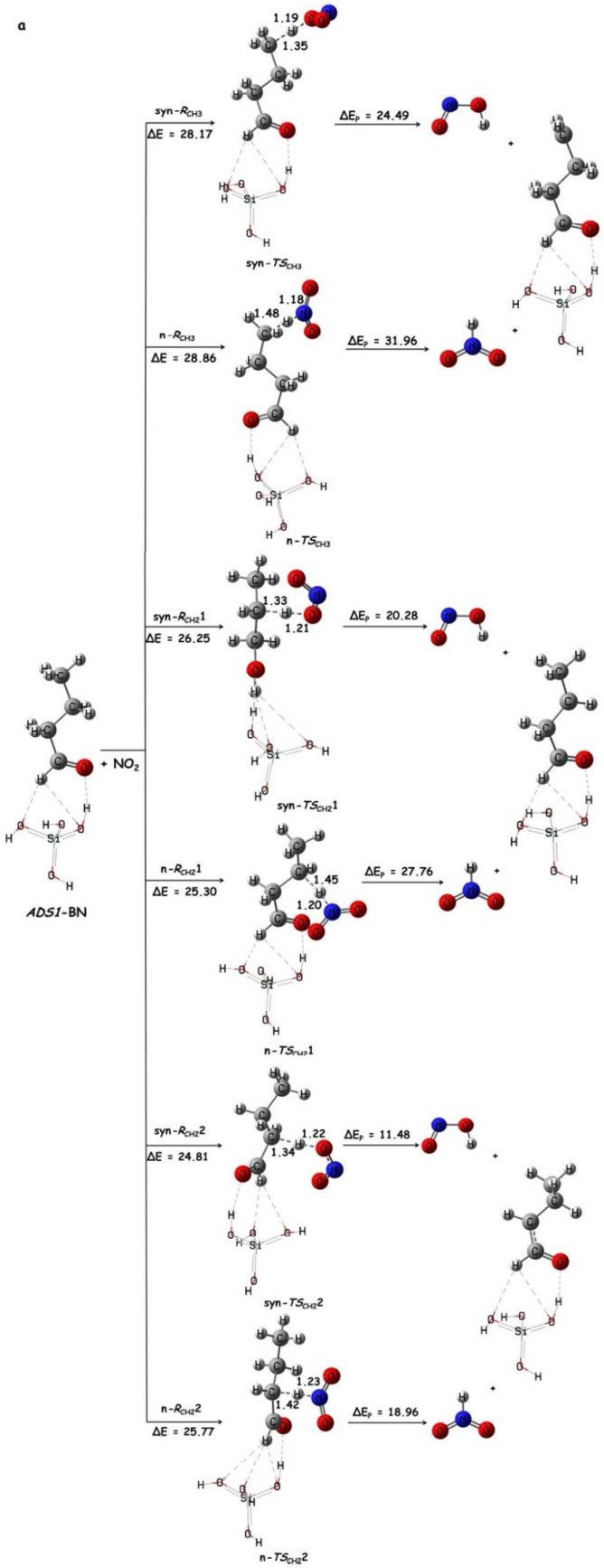


Fig. S6. The schematic diagram of heterogeneous reactions of NO_2 with propanal on the surface model embedded with the molecular structures (in Å) and the potential barriers (in kcal mol^{-1}).


a
ADS1-BN
+ NO2
syn-RCH3
ΔE = 28.17
ΔEp = 24.49
syn-TSCH3
n-RCH3
ΔE = 28.86
ΔEp = 31.96
n-TSCH3
syn-RCH21
ΔE = 26.25
ΔEp = 20.28
syn-TSCH21
n-RCH21
ΔE = 25.30
ΔEp = 27.76
n-TSCH21
syn-RCH22
ΔE = 24.81
ΔEp = 11.48
syn-TSCH22
n-RCH22
ΔE = 25.77
ΔEp = 18.96
n-TSCH22

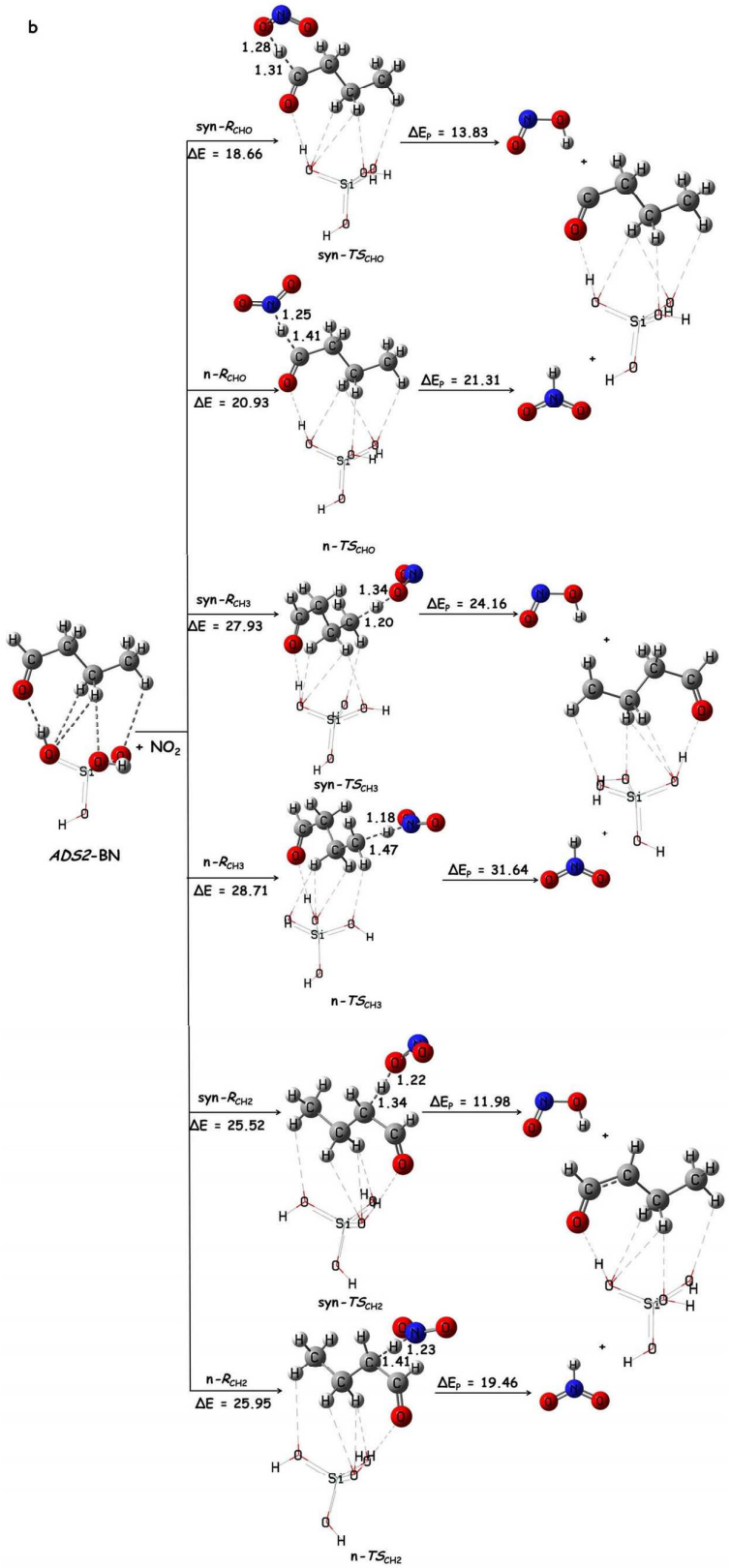


Fig. S7. The schematic diagram of heterogeneous reactions of NO_2 with butanal on the surface model embedded with the molecular structures (in Å) and the potential barriers (in kcal mol^{-1}).

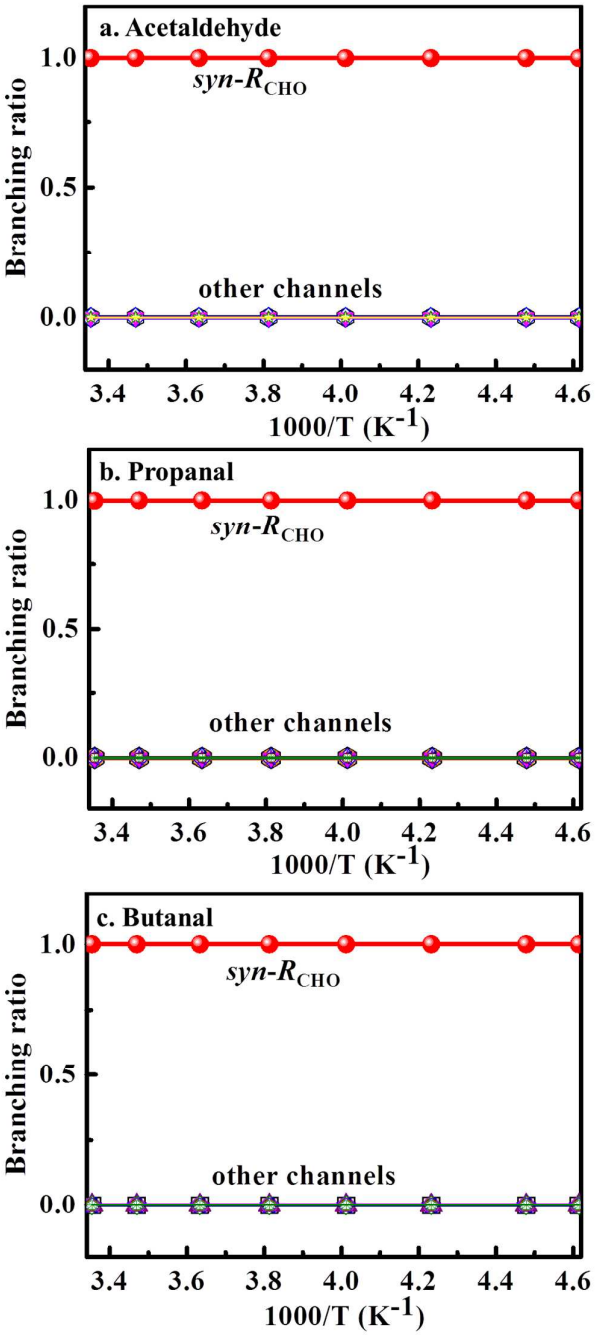


Fig. S8. Plot of calculated branching ratio versus 1000/T for the reaction of NO_2 with adsorbed acetaldehyde, propanal and butanal within the measured temperature range.

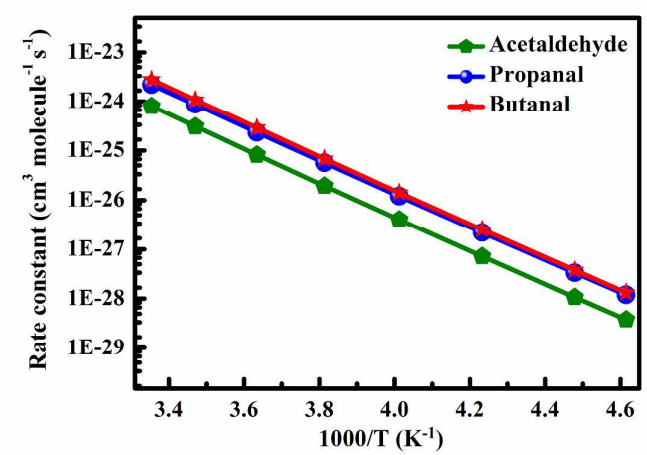


Fig. S9. Plot of calculated rate constants versus 1000/T for the heterogeneous reactions of NO_2 with three aldehydes within the measured temperature range.

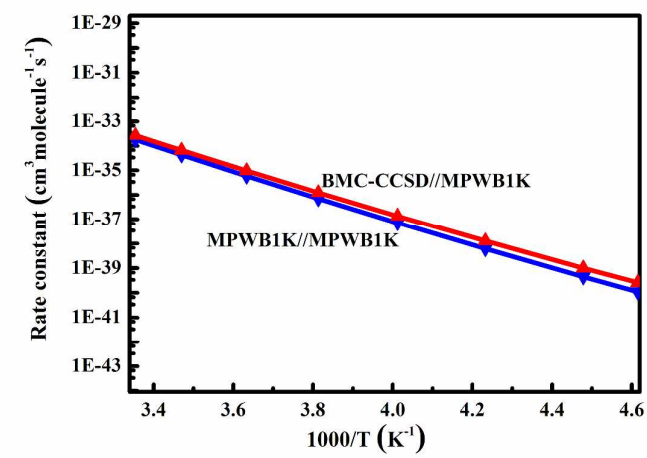
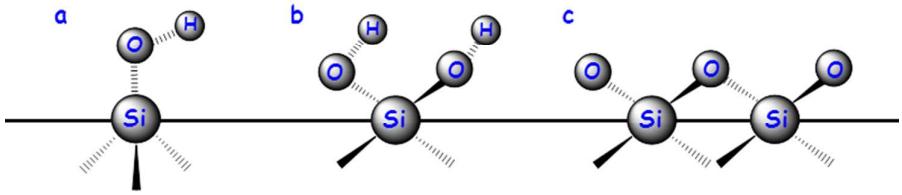


Fig. S10. The rate constants of *syn*-R_{CHO} channel in *Type 1* mechanism calculated by the BMC-CCSD//MPWB1K/6-311G(d,p) and MPWB1K/6-311G(3df,3pd)//MPWB1K/6-311G(d,p) levels.



Scheme S1 For silicic acid surface, the schematic diagram of (a) isolated silanol group (b) germinal silanol groups, and (c) siloxance bridge

Cartesian coordinates and ZPE of main species

Acetaldehyde ZPE = 0.056863

6	0	1.15572	-0.14607	-0.00002
1	0	1.69078	0.22055	-0.87331
1	0	1.13793	-1.2287	-0.00036
1	0	1.69037	0.2199	0.87383
6	0	-0.23311	0.39466	-0.00001
8	0	-1.21828	-0.275	0.
1	0	-0.30852	1.49668	0.00002

Propanal ZPE = 0.086283

6	0	0.54144	0.73244	0.00013
1	0	0.73485	1.36869	-0.865
1	0	0.73471	1.3684	0.86551
6	0	-0.91944	0.41993	-0.0001
8	0	-1.36732	-0.68489	0.00008
1	0	-1.59158	1.29591	-0.00052
6	0	1.40948	-0.5008	-0.00008
1	0	1.20472	-1.11203	-0.87263
1	0	2.46232	-0.2389	0.00005
1	0	1.2046	-1.11238	0.87221

Butanal ZPE = 0.115545

6	0	-2.279	-0.07036	0.00025
1	0	-2.53274	0.52105	-0.87658
1	0	-2.91671	-0.94907	-0.00017
1	0	-2.53216	0.5198	0.87808
6	0	-0.81559	-0.45354	-0.00046
1	0	-0.58332	-1.06953	0.8647
1	0	-0.584	-1.06846	-0.86659
6	0	0.09762	0.74902	-0.00009
1	0	-0.08302	1.38917	0.86648
1	0	-0.08377	1.39103	-0.86492
6	0	1.54916	0.3989	-0.00009
8	0	1.96981	-0.71693	0.00024
1	0	2.24408	1.25729	-0.00054

$ADC1^{\text{-Acetaldehyde}}_{\text{-Monomer}}$

14	0	1.361801	0.028973	0.024853
8	0	2.857307	-0.025264	-0.618539
1	0	3.206298	-0.888184	-0.807459
8	0	0.545461	-1.223880	-0.573057
1	0	-0.353906	-1.399589	-0.277910
8	0	1.305688	-0.046294	1.648555
1	0	1.588425	0.724153	2.125876
8	0	0.768952	1.501851	-0.380765
1	0	1.094375	1.860094	-1.198554
1	0	-1.631856	0.717433	-0.474160
8	0	-2.153619	-1.126697	0.065162
6	0	-2.420754	0.022360	-0.151756
6	0	-3.782960	0.591742	-0.003306
1	0	-3.754555	1.406499	0.716829
1	0	-4.100373	1.021639	-0.950741
1	0	-4.481643	-0.170001	0.317708

$ADC2^{\text{-Acetaldehyde}}_{\text{-Monomer}}$

14	0	1.286391	-0.027726	0.012509
8	0	2.688279	0.057642	-0.814312
1	0	2.874503	-0.660326	-1.407517
8	0	0.216235	-0.745944	-0.955107

1	0	-0.633951	-1.037823	-0.612727
8	0	1.353059	-0.859031	1.408703
1	0	1.750217	-0.420687	2.151335
8	0	0.934085	1.517826	0.418391
1	0	1.255518	2.183181	-0.178714
8	0	-2.395826	-1.193056	-0.047227
6	0	-3.070633	-0.211879	0.081609
6	0	-2.594241	1.181473	-0.103440
1	0	-1.534229	1.214042	-0.319286
1	0	-2.807413	1.755933	0.795153
1	0	-3.160302	1.641430	-0.911286
1	0	-4.131235	-0.324650	0.355314

$ADC1^{\text{-Acetaldehyde}}_{\text{-Trimer}}$

14	0	-0.274628	0.004245	1.596727
8	0	-1.695712	-0.251367	0.865851
8	0	-0.297967	-0.726218	3.044316
1	0	-0.762633	-1.550321	3.122980
8	0	0.891077	-0.523950	0.623147
8	0	0.032045	1.578739	1.855488
1	0	-0.378177	1.968359	2.618682
14	0	1.869187	-1.317186	-0.384065
14	0	-2.381056	-0.279169	-0.608144
8	0	-1.904852	-1.578209	-1.439020
1	0	-0.962499	-1.773826	-1.494373
8	0	-3.998940	-0.331089	-0.512647
1	0	-4.400730	-1.190882	-0.486733
8	0	-1.952642	1.144216	-1.284835
1	0	-2.364185	1.364085	-2.112321
8	0	0.840681	-1.947107	-1.504334
1	0	1.214968	-2.535389	-2.150606
8	0	2.982974	-0.339203	-0.997177
1	0	2.827312	0.617424	-1.002483
8	0	2.602776	-2.590227	0.305082
1	0	3.444257	-2.430222	0.715290
1	0	0.419487	1.866743	-1.017738
6	0	1.196225	2.599249	-0.765781
8	0	2.359598	2.298970	-0.798381
6	0	0.705867	3.947406	-0.399454
1	0	0.106406	4.350602	-1.212348
1	0	0.049321	3.838536	0.459483
1	0	1.532566	4.608079	-0.171610

$ADC2^{\text{-Acetaldehyde}}_{\text{-Trimer}}$

14	0	-0.281457	0.376191	1.527036
8	0	-1.714593	0.038678	0.859529
8	0	-0.322719	-0.083113	3.081371
1	0	-0.868532	-0.826079	3.308197
8	0	0.869406	-0.356754	0.674686
8	0	0.085375	1.956793	1.473002
1	0	-0.376333	2.529351	2.073819
14	0	1.739712	-1.380532	-0.212432
14	0	-2.545714	-0.121016	-0.527429
8	0	-2.011272	-1.390459	-1.370037
1	0	-1.062936	-1.541534	-1.446671
8	0	-4.127070	-0.358545	-0.252300
1	0	-4.416567	-1.259640	-0.177623
8	0	-2.370753	1.315563	-1.277167
1	0	-2.902615	1.468904	-2.048724

8	0	0.744699	-1.741634	-1.474450
1	0	1.055792	-2.393852	-2.092663
8	0	3.130132	-0.716003	-0.665570
1	0	3.219436	0.246849	-0.629612
8	0	2.045566	-2.788434	0.534979
1	0	2.857612	-2.844164	1.024656
6	0	2.042257	2.575511	-0.716344
8	0	3.042061	1.997368	-0.389834
1	0	1.834565	3.566302	-0.290754
6	0	1.048494	2.074012	-1.694331
1	0	0.063226	2.048934	-1.236651
1	0	0.991707	2.780070	-2.521262
1	0	1.317909	1.095046	-2.072766

$ADCI^{\text{Acetaldehyde}}_{\text{-Hexamer}}$

14	0	-1.056050	2.617346	-0.538339
14	0	1.843198	2.599140	0.325878
14	0	3.324520	-0.012525	0.704870
14	0	1.863238	-2.628242	0.246726
14	0	-1.074905	-2.582441	-0.498673
14	0	-2.547817	0.013314	-0.972214
8	0	0.230248	2.689866	0.440326
8	0	2.454764	1.304914	1.077342
8	0	2.545584	-1.389077	1.038492
8	0	0.259369	-2.681232	0.420208
8	0	-1.949565	-1.268989	-0.164078
8	0	-2.019844	1.358999	-0.216383
8	0	-0.540107	2.374041	-2.074416
1	0	0.403809	2.499098	-2.204791
8	0	-1.850751	4.009390	-0.331824
1	0	-2.740951	4.085390	-0.652869
8	0	2.148598	2.465239	-1.278478
1	0	2.785814	1.783352	-1.509788
8	0	2.520438	3.893824	1.013572
1	0	2.075553	4.730802	0.961824
8	0	3.562648	0.066437	-0.913578
1	0	3.309973	-0.727232	-1.394061
8	0	4.696678	-0.011154	1.553897
1	0	5.020819	0.810106	1.902154
8	0	2.211960	-2.357166	-1.331716
1	0	1.470335	-2.481221	-1.930845
8	0	2.441906	-4.024901	0.812863
1	0	3.339507	-4.063569	1.119015
8	0	-0.506890	-2.469127	-2.032852
1	0	-0.948787	-1.815248	-2.580813
8	0	-2.013342	-3.868489	-0.234275
1	0	-1.609180	-4.720631	-0.126567
8	0	-1.911284	-0.051507	-2.474144
1	0	-1.453699	0.746874	-2.749186
8	0	-4.147151	-0.018567	-1.031770
1	0	-4.611346	-0.044906	-0.186042
1	0	-3.015152	-0.193283	2.044081
6	0	-4.047733	-0.082277	2.403097
8	0	-4.954663	0.001222	1.622021
6	0	-4.226148	-0.046287	3.874709
1	0	-3.828314	-0.961861	4.306640
1	0	-3.642711	0.773807	4.287297
1	0	-5.271728	0.067835	4.129988

ADC2-Acetaldehyde-Hexamer

14	0	1.568280	-2.357841	-0.554270
14	0	-1.354917	-2.701334	0.143034
14	0	-3.284691	-0.400127	0.392387
14	0	-2.119882	2.377241	0.146038
14	0	0.861446	2.713568	-0.210245
14	0	2.781764	0.425320	-0.651268
8	0	0.245658	-2.569740	0.356567
8	0	-2.171636	-1.495923	0.843816
8	0	-2.813400	1.085695	0.837277
8	0	-0.566247	2.555338	0.549311
8	0	1.868374	1.508047	0.151674
8	0	2.428968	-1.069031	-0.105577
8	0	1.112103	-2.049807	-2.096161
1	0	0.210225	-2.304524	-2.307858
8	0	2.437905	-3.710965	-0.383902
1	0	3.338592	-3.719236	-0.684334
8	0	-1.568249	-2.611934	-1.479529
1	0	-2.309240	-2.070554	-1.763619
8	0	-1.896319	-4.071162	0.805685
1	0	-1.393184	-4.869003	0.697211
8	0	-3.391272	-0.451343	-1.235319
1	0	-3.126581	0.363584	-1.672907
8	0	-4.708979	-0.774180	1.050328
1	0	-4.723283	-1.332927	1.817616
8	0	-2.217654	2.078607	-1.462878
1	0	-1.432951	2.330142	-1.960337
8	0	-2.870181	3.729666	0.612701
1	0	-3.818253	3.742436	0.658219
8	0	0.488998	2.630827	-1.806125
1	0	1.094286	2.092082	-2.324398
8	0	1.565146	4.097269	0.230513
1	0	1.027872	4.869916	0.355075
8	0	2.308218	0.522290	-2.216232
1	0	1.952644	-0.292495	-2.577542
8	0	4.352365	0.751921	-0.561445
1	0	4.683971	0.802984	0.332893
6	0	3.245334	-0.165850	3.051214
1	0	3.738798	-0.567505	3.951641
8	0	3.916773	0.295669	2.174240
6	0	1.765463	-0.258139	3.033092
1	0	1.366215	0.115691	3.972799
1	0	1.350681	0.285222	2.195471
1	0	1.482834	-1.307406	2.965209

ADC1-Propanal-Monomer

14	0	1.846126	0.003266	0.045564
8	0	3.362826	-0.075472	-0.543869
1	0	3.681603	-0.938863	-0.778496
8	0	1.002561	-1.168615	-0.667531
1	0	0.086007	-1.323770	-0.417502
8	0	1.721472	-0.179003	1.656837
1	0	2.015272	0.544615	2.196661
8	0	1.333562	1.525368	-0.278564
1	0	1.704115	1.921878	-1.058610
1	0	-1.102781	0.859280	-0.519720
8	0	-1.713291	-0.995118	-0.119693
6	0	-1.927382	0.176550	-0.268299

6	0	-3.275688	0.787397	-0.121885
1	0	-3.183604	1.575717	0.627063
1	0	-3.488374	1.313663	-1.053968
6	0	-4.353792	-0.206904	0.229034
1	0	-5.315244	0.284256	0.333688
1	0	-4.120673	-0.712262	1.160128
1	0	-4.437961	-0.969782	-0.537662

ADC2-Propanal-Monomer

14	0	1.608403	-0.039521	0.023104
8	0	3.123490	-0.590244	-0.220643
1	0	3.220199	-1.534747	-0.251111
8	0	0.614610	-1.104152	-0.664431
1	0	-0.307294	-1.173382	-0.405337
8	0	1.173268	0.117039	1.587441
1	0	1.535969	0.859394	2.055621
8	0	1.589354	1.473054	-0.589818
1	0	2.107177	1.615878	-1.372916
8	0	-2.116586	-1.436763	-0.051535
6	0	-3.106330	-0.772680	0.056912
6	0	-3.145623	0.714022	0.006490
6	0	-1.792254	1.357730	-0.156759
1	0	-3.651634	1.045899	0.914653
1	0	-3.828650	0.978332	-0.803281
1	0	-4.077328	-1.271725	0.203357
1	0	-1.878963	2.437421	-0.207347
1	0	-1.301465	1.018513	-1.062648
1	0	-1.143505	1.111804	0.677582

ADC1-Propanal-Trimer

14	0	0.411856	-0.110350	1.594424
8	0	1.550332	-0.997145	0.863280
8	0	0.974446	0.377625	3.035122
1	0	1.897100	0.588533	3.108972
8	0	0.014622	1.097301	0.609737
8	0	-0.956889	-0.941196	1.871375
1	0	-0.987132	-1.451623	2.671947
14	0	-0.047144	2.363580	-0.386466
14	0	2.076926	-1.457838	-0.604150
8	0	2.737558	-0.215720	-1.395814
1	0	2.244736	0.609683	-1.463481
8	0	3.207384	-2.615136	-0.494886
1	0	4.111421	-2.329627	-0.444696
8	0	0.759736	-2.092067	-1.330898
1	0	0.897826	-2.529038	-2.162926
8	0	1.141619	2.051705	-1.481251
1	0	1.327356	2.730108	-2.120861
8	0	-1.508421	2.511354	-1.031599
1	0	-2.100532	1.744353	-1.034103
8	0	0.366049	3.763015	0.324334
1	0	-0.334826	4.265090	0.722665
1	0	-1.382985	-0.921604	-0.943586
6	0	-2.456496	-0.820815	-0.743672
8	0	-3.005166	0.246156	-0.828677
6	0	-3.163271	-2.073604	-0.375457
1	0	-2.615673	-2.482441	0.473032
1	0	-2.998258	-2.781690	-1.189289
6	0	-4.628071	-1.874686	-0.078823
1	0	-4.758951	-1.185450	0.748789

1	0	-5.141375	-1.449191	-0.934872
1	0	-5.104785	-2.815112	0.177040

ADC2-Propanal-Trimer

14	0	0.361587	0.249078	1.560351
8	0	1.692881	0.682632	0.728725
8	0	0.415144	0.752777	3.093207
1	0	0.164548	1.647588	3.285120
8	0	-0.916255	0.917587	0.825484
8	0	0.270922	-1.371490	1.539333
1	0	1.015609	-1.779832	1.094264
14	0	-1.709616	1.543831	-0.431037
14	0	2.567801	0.083813	-0.496301
8	0	1.997012	0.640532	-1.898592
1	0	1.095948	0.982815	-1.888174
8	0	4.152486	0.403979	-0.405786
1	0	4.459950	1.212654	-0.796969
8	0	2.414977	-1.542031	-0.298719
1	0	3.037616	-2.107786	-0.739395
8	0	-0.597524	1.651790	-1.643271
1	0	-0.834911	2.222771	-2.366284
8	0	-2.987242	0.637959	-0.801101
1	0	-3.002038	-0.268892	-0.473560
8	0	-2.213910	3.066862	-0.178383
1	0	-3.096170	3.170058	0.158127
6	0	-2.070745	-2.782540	0.397890
8	0	-2.820809	-1.847957	0.392247
1	0	-2.092942	-3.486937	1.241132
6	0	-1.113638	-3.106758	-0.695991
1	0	-0.168722	-3.385959	-0.234022
1	0	-1.488918	-4.019948	-1.164198
6	0	-0.940988	-1.993651	-1.696506
1	0	-0.532386	-1.117507	-1.205267
1	0	-1.887675	-1.708550	-2.143195
1	0	-0.255962	-2.278015	-2.487283

ADC1-Propanal-Hexamer

14	0	-1.133856	2.357787	-0.917429
14	0	1.612123	2.814423	0.264695
14	0	3.344445	0.438026	0.983957
14	0	2.303753	-2.375672	0.571321
14	0	-0.479033	-2.797631	-0.557372
14	0	-2.186147	-0.445083	-1.376414
8	0	0.000295	2.660854	0.196029
8	0	2.314261	1.675600	1.172760
8	0	2.679749	-0.993115	1.331778
8	0	0.715791	-2.663072	0.533557
8	0	-1.562980	-1.609478	-0.423742
8	0	-1.942169	0.985566	-0.631778
8	0	-0.404461	2.129474	-2.367003
1	0	0.523138	2.381239	-2.391020
8	0	-2.137599	3.624118	-0.886040
1	0	-2.984833	3.552920	-1.308505
8	0	2.125346	2.636595	-1.281361
1	0	2.850228	2.014484	-1.393576
8	0	2.000894	4.238277	0.918586
1	0	1.423292	4.979851	0.786329
8	0	3.742235	0.456056	-0.605396
1	0	3.681285	-0.398025	-1.043428

8	0	4.608747	0.622462	1.970580
1	0	4.884701	1.498502	2.209980
8	0	2.831162	-2.165799	-0.966304
1	0	2.195029	-2.420810	-1.640827
8	0	2.991997	-3.621177	1.333104
1	0	3.814504	-3.487148	1.787485
8	0	0.274347	-2.673112	-2.008590
1	0	-0.159604	-2.093031	-2.640786
8	0	-1.260654	-4.191777	-0.336763
1	0	-0.763316	-4.971549	-0.123167
8	0	-1.330040	-0.494470	-2.766235
1	0	-0.968690	0.351449	-3.042645
8	0	-3.745597	-0.674280	-1.662293
1	0	-4.323431	-0.608952	-0.893758
1	0	-3.006526	-0.597031	1.584783
6	0	-4.048501	-0.302757	1.770784
8	0	-4.838204	-0.259857	0.867410
6	0	-4.394878	0.028274	3.178037
1	0	-3.705932	0.813723	3.493180
1	0	-4.121249	-0.838598	3.781842
6	0	-5.836961	0.424333	3.371194
1	0	-6.038566	0.654096	4.411897
1	0	-6.080007	1.296102	2.773038
1	0	-6.500930	-0.375129	3.060108

$ADC2_{\text{-Hexamer}}^{\text{-Propanal}}$

14	0	-1.130315	2.549032	-0.747461
14	0	1.734355	2.636558	0.220935
14	0	3.319293	0.098750	0.668703
14	0	1.966859	-2.569930	0.191618
14	0	-0.959964	-2.624010	-0.583252
14	0	-2.556563	-0.111731	-1.083991
8	0	0.116099	2.655709	0.279975
8	0	2.377720	1.376802	1.004273
8	0	2.596897	-1.310035	0.995141
8	0	0.365109	-2.684491	0.353058
8	0	-1.872242	-1.336595	-0.260447
8	0	-2.104941	1.305206	-0.421654
8	0	-0.555125	2.253111	-2.252514
1	0	0.384754	2.417228	-2.363459
8	0	-1.927778	3.950700	-0.620479
1	0	-2.805840	4.012506	-0.976196
8	0	2.102250	2.505632	-1.370344
1	0	2.777505	1.851923	-1.573278
8	0	2.328853	3.965280	0.921472
1	0	1.848037	4.780226	0.844633
8	0	3.602659	0.172446	-0.942615
1	0	3.372782	-0.627351	-1.424818
8	0	4.665899	0.177365	1.554612
1	0	4.927808	1.015323	1.915212
8	0	2.317603	-2.277484	-1.382425
1	0	1.583262	-2.421054	-1.987008
8	0	2.595072	-3.946750	0.754719
1	0	3.492474	-3.952158	1.063747
8	0	-0.373814	-2.493903	-2.110336
1	0	-0.857054	-1.877027	-2.667369
8	0	-1.861869	-3.940590	-0.335932
1	0	-1.430378	-4.780014	-0.234289

8	0	-1.936062	-0.192494	-2.597049
1	0	-1.479373	0.602318	-2.881899
8	0	-4.155041	-0.249978	-1.155766
1	0	-4.590607	-0.299417	-0.305735
6	0	-4.338280	-0.105859	2.835563
1	0	-5.292306	-0.212742	3.377149
8	0	-4.330988	-0.113012	1.639082
6	0	-3.127507	0.042140	3.686486
1	0	-3.119982	-0.812584	4.365693
1	0	-3.305302	0.904937	4.331754
6	0	-1.837205	0.161952	2.915014
1	0	-0.995191	0.259331	3.592109
1	0	-1.678414	-0.710160	2.291745
1	0	-1.847937	1.022609	2.255713

$ADC1_{\text{-Monomer}}^{\text{-Butanal}}$

14	0	2.370030	0.035625	0.064693
8	0	3.895792	-0.014398	-0.504419
1	0	4.248756	-0.875381	-0.694716
8	0	1.579323	-1.199460	-0.600763
1	0	0.663738	-1.373315	-0.359086
8	0	2.233019	-0.074950	1.681403
1	0	2.488430	0.685844	2.188641
8	0	1.806365	1.520682	-0.337848
1	0	2.177180	1.895287	-1.128535
1	0	-0.594426	0.747222	-0.634386
8	0	-1.150560	-1.095016	-0.117953
6	0	-1.401256	0.055737	-0.350972
6	0	-2.770709	0.628923	-0.270600
1	0	-2.721988	1.474619	0.419076
1	0	-2.988331	1.077547	-1.242694
6	0	-3.832640	-0.364018	0.136868
1	0	-3.558985	-0.795669	1.096315
1	0	-3.829554	-1.191384	-0.568369
6	0	-5.208264	0.260850	0.211656
1	0	-5.508538	0.671049	-0.749772
1	0	-5.955969	-0.469098	0.505768
1	0	-5.235043	1.070718	0.936988

$ADC2_{\text{-Monomer}}^{\text{-Butanal}}$

14	0	1.787967	-0.055552	0.024700
8	0	3.357234	-0.361627	-0.293092
1	0	3.590751	-1.277881	-0.384614
8	0	0.937350	-1.213614	-0.702197
1	0	0.039471	-1.429194	-0.438416
8	0	1.390645	-0.053796	1.605917
1	0	1.655503	0.705909	2.110333
8	0	1.531915	1.473068	-0.492614
1	0	1.999447	1.733523	-1.277241
8	0	-1.716499	-1.975875	-0.090143
6	0	-2.781912	-1.445939	0.043593
6	0	-3.003531	0.025039	0.049359
6	0	-1.736764	0.832968	-0.090467
1	0	-3.538607	0.264724	0.971126
1	0	-3.716525	0.242582	-0.749683
1	0	-3.680956	-2.068925	0.173154
1	0	-1.234679	0.549317	-1.011773
1	0	-1.060728	0.560621	0.716658
6	0	-1.975851	2.325152	-0.078006

1	0	-2.446634	2.644281	0.849211
1	0	-1.033469	2.853388	-0.176379
1	0	-2.621914	2.630816	-0.898018

$ADC1_{\text{-Trimer}}^{\text{-Butanal}}$

14	0	0.595753	-0.215672	1.591570
8	0	1.297398	-1.481421	0.869577
8	0	1.289726	0.012248	3.039630
1	0	2.218783	-0.163797	3.123953
8	0	0.723738	1.048061	0.604850
8	0	-0.993381	-0.432291	1.849675
1	0	-1.234996	-0.887861	2.647413
14	0	1.169542	2.258909	-0.360980
14	0	1.647131	-2.091720	-0.596167
8	0	2.739099	-1.178663	-1.357787
1	0	2.589656	-0.229848	-1.436880
8	0	2.266878	-3.586101	-0.483593
1	0	3.211722	-3.654851	-0.421395
8	0	0.204977	-2.186622	-1.354480
1	0	0.187713	-2.642440	-2.187674
8	0	2.121403	1.520815	-1.482105
1	0	2.554362	2.078495	-2.118702
8	0	-0.113365	3.001790	-0.975728
1	0	-0.952432	2.521098	-1.015894
8	0	2.115049	3.355081	0.372369
1	0	1.678300	4.086078	0.792947
1	0	-1.298399	-0.239588	-1.029707
6	0	-2.259759	0.250332	-0.830521
8	0	-2.369442	1.446526	-0.893675
6	0	-3.383322	-0.658238	-0.491536
1	0	-3.036576	-1.255309	0.352800
1	0	-3.485237	-1.366653	-1.316816
6	0	-4.682791	0.048842	-0.192442
1	0	-4.516910	0.752210	0.619851
1	0	-4.964972	0.652868	-1.051430
6	0	-5.795405	-0.912957	0.162157
1	0	-5.539772	-1.505459	1.037615
1	0	-6.719042	-0.385178	0.379656
1	0	-5.995137	-1.604259	-0.653477

$ADC2_{\text{-Trimer}}^{\text{-Butanal}}$

14	0	0.770840	0.454178	1.533854
8	0	2.109041	0.450588	0.604666
8	0	1.028367	1.168953	2.959567
1	0	1.046573	2.117050	2.993241
8	0	-0.378906	1.276836	0.735856
8	0	0.308753	-1.076653	1.784999
1	0	0.917951	-1.733106	1.443796
14	0	-1.004274	1.847382	-0.636322
14	0	2.812360	-0.564289	-0.444641
8	0	2.245580	-0.281294	-1.931859
1	0	1.392965	0.165702	-1.965753
8	0	4.428362	-0.477052	-0.478961
1	0	4.817823	0.155622	-1.070372
8	0	2.420917	-2.041041	0.154892
1	0	2.835382	-2.811172	-0.214753
8	0	-0.241958	1.012981	-1.839989
1	0	-0.502769	1.250737	-2.723907
8	0	-2.603719	1.701474	-0.678356

1	0	-3.078574	0.976867	-0.257711
8	0	-0.661263	3.415650	-0.881596
1	0	-1.314879	4.040702	-0.591326
6	0	-4.144024	-1.484975	0.609633
8	0	-4.144341	-0.290744	0.507975
1	0	-4.962909	-1.976402	1.157104
6	0	-3.104256	-2.385144	0.047159
1	0	-2.706937	-2.966975	0.881940
1	0	-3.616223	-3.113448	-0.586092
6	0	-2.001564	-1.662689	-0.686135
1	0	-1.553983	-0.954225	0.002610
1	0	-2.427041	-1.081170	-1.501685
6	0	-0.931246	-2.594862	-1.204164
1	0	-1.335179	-3.313796	-1.913625
1	0	-0.142584	-2.039961	-1.702098
1	0	-0.474708	-3.149769	-0.388340
$ADCI^{\text{-Butanal}}_{\text{-Hexamer}}$				
14	0	-0.341294	2.727725	-0.937193
14	0	2.111136	2.432279	0.809546
14	0	3.313754	-0.263497	1.463873
14	0	1.926208	-2.722905	0.367143
14	0	-0.660691	-2.391995	-1.176705
14	0	-1.842908	0.283054	-1.919148
8	0	0.552331	2.608432	0.406831
8	0	2.397204	1.066729	1.626747
8	0	2.427598	-1.616385	1.439960
8	0	0.340666	-2.644789	0.074846
8	0	-1.505223	-1.027698	-1.009439
8	0	-1.497027	1.601703	-1.024832
8	0	0.616741	2.450092	-2.236776
1	0	1.559503	2.509550	-2.060649
8	0	-0.991454	4.207464	-0.907732
1	0	-1.719060	4.403183	-1.485340
8	0	2.911602	2.364394	-0.618565
1	0	3.577989	1.673490	-0.671556
8	0	2.579134	3.646116	1.766637
1	0	2.214904	4.511611	1.626867
8	0	4.067302	-0.119186	0.017946
1	0	3.904205	-0.846880	-0.589492
8	0	4.346860	-0.353152	2.699559
1	0	4.455830	0.405558	3.259279
8	0	2.731943	-2.357684	-1.012955
1	0	2.191468	-2.384217	-1.807800
8	0	2.223977	-4.207491	0.927889
1	0	3.008808	-4.360946	1.439204
8	0	0.334994	-2.246129	-2.472060
1	0	0.078456	-1.564634	-3.099219
8	0	-1.717096	-3.607182	-1.287033
1	0	-1.415261	-4.497131	-1.152717
8	0	-0.837508	0.227857	-3.205484
1	0	-0.234194	0.972362	-3.266244
8	0	-3.372408	0.293330	-2.397744
1	0	-3.999562	0.222663	-1.670930
1	0	-2.706032	0.074847	1.095414
6	0	-3.801946	0.039547	1.161308
8	0	-4.471297	0.124417	0.168761
6	0	-4.377546	-0.121086	2.522863

1	0	-3.985503	0.694427	3.134898
1	0	-3.935272	-1.024194	2.949465
6	0	-5.886428	-0.170174	2.554007
1	0	-6.277743	0.740114	2.106570
1	0	-6.224529	-0.981345	1.914112
6	0	-6.429856	-0.343751	3.955123
1	0	-7.514959	-0.377231	3.953984
1	0	-6.072111	-1.266771	4.405284
1	0	-6.125864	0.476376	4.601391

ADC2-Butanal-Hexamer

14	0	-0.722439	2.694510	-0.587885
14	0	2.110876	2.635250	0.473974
14	0	3.485789	-0.032463	0.883392
14	0	2.088364	-2.628918	0.205532
14	0	-0.747619	-2.531034	-0.860536
14	0	-2.168591	0.111068	-1.250385
8	0	0.493402	2.723529	0.478729
8	0	2.674322	1.324644	1.235887
8	0	2.603977	-1.370760	1.091866
8	0	0.478159	-2.754618	0.179789
8	0	-1.619007	-1.225199	-0.501888
8	0	-1.694929	1.416555	-0.396716
8	0	-0.102023	2.538810	-2.096478
1	0	0.851303	2.647666	-2.150432
8	0	-1.542941	4.069760	-0.365733
1	0	-2.407411	4.157766	-0.748005
8	0	2.529925	2.534582	-1.106548
1	0	3.157971	1.835643	-1.310534
8	0	2.729903	3.920172	1.230746
1	0	2.241912	4.734322	1.226545
8	0	3.862898	0.101689	-0.705621
1	0	3.688804	-0.687578	-1.227143
8	0	4.772662	-0.169914	1.849320
1	0	5.212142	0.616673	2.147921
8	0	2.605672	-2.326728	-1.319173
1	0	1.915927	-2.376163	-1.988063
8	0	2.680832	-3.997293	0.822652
1	0	3.443565	-3.952144	1.385700
8	0	-0.012663	-2.301522	-2.309255
1	0	-0.404912	-1.607407	-2.845750
8	0	-1.739758	-3.804191	-0.817291
1	0	-1.368173	-4.677358	-0.791124
8	0	-1.423885	0.121032	-2.706651
1	0	-0.974982	0.942540	-2.919642
8	0	-3.756240	0.096311	-1.435436
1	0	-4.362734	0.254983	-0.705220
6	0	-5.780504	0.440185	1.757319
1	0	-6.713296	0.783513	2.230925
8	0	-5.602558	0.659941	0.592523
6	0	-4.825248	-0.275987	2.642571
1	0	-5.362205	-1.130131	3.062473
1	0	-4.630607	0.375545	3.497576
6	0	-3.551100	-0.698847	1.954116
1	0	-3.799943	-1.323138	1.099790
1	0	-3.058280	0.184813	1.553620
6	0	-2.598263	-1.436995	2.866133
1	0	-1.692262	-1.701996	2.331303

1	0	-2.313845	-0.826477	3.720044
1	0	-3.043590	-2.353401	3.246145

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