ADDITIONS AND CORRECTIONS

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J. A. D. Grabowy and P. M. Mayer*: Entropy changes in the dissociation of proton-bound complexes: A variational RRKM study

The variational RRKM modeling of $\Delta S^{\ddagger}$ for the dissociation of the two proton-bound pairs $(CH_3CN)(CH_3CH_2CH_2OH)H^+$ and $(CH_3CN)((CH_3)_2CHOH)H^+$ was carried out for the dissociation channels leading to $CH_3CNH^+ + CH_3CH_2$-

TABLE 1: Calculated Vibrational Frequencies for Proton-Bound Acetonitrile−Alcohol Pairs, Transition States, and Their Dissociation Products

	harmonic frequencies (cm^{-1})[a]
$(CH_3CN)(CH_3OH)H^+$	67, 80, 129, 147, 260, 329, 331, 517, 882, 908, 964, 1013, 1015, 1098, 1160, 1290, 1374, 1417, 1417, 1419, 1451, 1454, 1665, 1943, 2155, 2943, 2983, 3039, 3040, 3103, 3117, 3470
CH_3CNH^+	322, 322, 541, 541, 866, 1008, 1008, 1362, 1394, 1394, 2183, 2927, 3029, 3029, 3486
CH_3OH	313, 1004, 1028, 1129, 1306, 1437, 1464, 1473, 2908, 2977, 3045, 3562
transition state (common)	325, 327, 415, 711, 725, 984, 1010, 1011, 1063, 1209, 1233, 1265, 1368, 1405, 1406, 1428, 1459, 1462, 2169, 2714, 2935, 2946, 3034, 3034, 3047, 3074, 3516
transition state (vanishing)[b]	67, 80, 129, 147
α values	0.46, 0.44, 0.20, 0.20
rotational constant for rotor (GHz)	23.3
moment of inertia (10^{-47} kg m^{-2})	360, 643, 667 for $(CH_3CN)(CH_3OH)H^+$ 5.39, 99.4, 99.4 for CH_3CNH^+ 6.61, 34.3, 35.5 for CH_3OH
$(CH_3CN)(CH_3CH_2OH)H^+$	36, 51, 88, 125, 207, 251, 328, 329, 408, 512, 783, 790, 900, 950, 970, 1014, 1015, 1066, 1157, 1223, 1268, 1396, 1418, 1419, 1446, 1456, 1473, 1664, 2144, 2159, 2937, 2943, 2991, 3019, 3039, 3039, 3040, 3073, 3455
CH_3CNH^+	322, 322, 541, 541, 866, 1008, 1008, 1362, 1394, 1394, 2183, 2927, 3029, 3029, 3486
CH_3CH_2OH	225, 279, 401, 794, 871, 1009, 1058, 1140, 1214, 1248, 1362, 1404, 1445, 1461, 1490, 2896, 2930, 2939, 3014, 3026, 3546
transition state (common)	265, 325, 326, 404, 527, 587, 792, 827, 989, 883, 1011, 1011, 1062, 1103, 1149, 1219, 1258, 1366, 1368, 1400, 1406, 1406, 1446, 1459, 1481, 2164, 2923, 2934, 2935, 2965, 2984, 3017, 3033, 3034, 3034, 3501
transition state (vanishing)[b]	36, 51, 88, 125
α values	0.27, 0.31, 0.25, 0.25
rotational constant for rotor (GHz)	19.7
moment of inertia (10^{-47} kg m^{-2})	42.6, 1030, 1050 for $(CH_3CN)(CH_3CH_2OH)H^+$ 5.39, 99.4, 99.4 for CH_3CNH^+ 24.2, 89.3, 103 for CH_3CH_2OH
$(CH_3CN)(CH_3CH_2CH_2OH)H^+$	33, 40, 86, 111, 121, 186, 225, 286, 328, 329, 434, 511, 746, 825, 864, 893, 903, 969, 1013, 1015, 1017, 1087, 1158, 1204, 1247, 1279, 1310, 1374, 1375, 1395, 1419, 1419, 1456, 1461, 1466, 1472, 1663, 2146, 2193, 2926, 2936, 2943, 2979, 2989, 3019, 3032, 3040, 3040, 3063, 3452
$CH_3CH_2CH_2OH$	115, 225, 246, 265, 439, 741, 865, 872, 1003, 1036, 1051, 1144, 1205, 1220, 1269, 1299, 1383, 1400, 1458, 1462, 1468, 1487, 2883, 2917, 2927, 2934, 2979, 3000, 3005, 3542
CH_3CNH^+	322, 322, 541, 541, 866, 1008, 1008, 1362, 1394, 1394, 2183, 2927, 3029, 3029, 3486
transition state (common)	122, 210, 265, 319, 320, 417, 561, 617, 740, 791, 865, 895, 928, 1017, 1018, 1048, 1145, 1188, 1241, 1284, 1306, 1371, 1377, 1398, 1428, 1428, 1461, 1464, 1470, 1477, 1638, 2118, 2567, 2938, 2943, 2966, 2993, 3013, 3034, 3036, 3036, 3058, 3218, 3461
transition state (vanishing)[b]	33, 40, 86, 111
α values	0.13, 0.09, 0.03, 0.08
rotational constant for rotor (GHz)	10.6
moment of inertia (10^{-47} kg m^{-2})	78.8, 1460, 1510 for $(CH_3CN)(CH_3CH_2CH_2OH)H^+$ 5.39, 99.4, 99.4 for CH_3CNH^+ 31.7, 220, 236 for $CH_3CH_2CH_2OH$
$(CH_3CN)((CH_3)_2CHOH)H^+$	6, 36, 47, 89, 116, 197, 219, 265, 329, 330, 352, 388, 449, 510, 706, 875, 898, 916, 920, 954, 1014, 1015, 1064, 1109, 1175, 1235, 1308, 1355, 1374, 1395, 1396, 1419, 1420, 1438, 1446, 1456, 1464, 1671, 2141, 2348, 2930, 2937, 2943, 2980, 3015, 3026, 3031, 3036, 3039, 3040, 3445
$(CH_3)_2CHOH$	216, 266, 290, 350, 398, 465, 799, 902, 925, 938, 1054, 1117, 1157, 1226, 1326, 1350, 1378, 1391, 1444, 1446, 1458, 1467, 2883, 2912, 2925, 2991, 3007, 3012, 3020, 3529
CH_3CNH^+	322, 322, 541, 541, 866, 1008, 1008, 1362, 1394, 1394, 2183, 2927, 3029, 3029, 3486
transition state (common)	225, 267, 320, 320, 347, 349, 371, 438, 657, 809, 887, 892, 907, 936, 995, 1017, 1018, 1095, 1166, 1215, 1311, 1353, 1377, 1394, 1399, 1428, 1428, 1440, 1450, 1461, 1468, 1642, 2116, 2859, 2934, 2940, 2943, 3000, 3020, 3027, 3035, 3035, 3036
transition state (vanishing)[b]	36, 47, 89, 116
α values	0.13, 0.17, 0.05, 0.09
rotational constant for rotor (GHz)	7.0
moment of inertia (10^{-47} kg m^{-2})	120, 1130, 1200 for $(CH_3CN)((CH_3)_2CHOH)H^+$ 5.39, 99.4, 99.4 for CH_3CNH^+ 96.9, 104, 176 for $(CH_3)_2CHOH$

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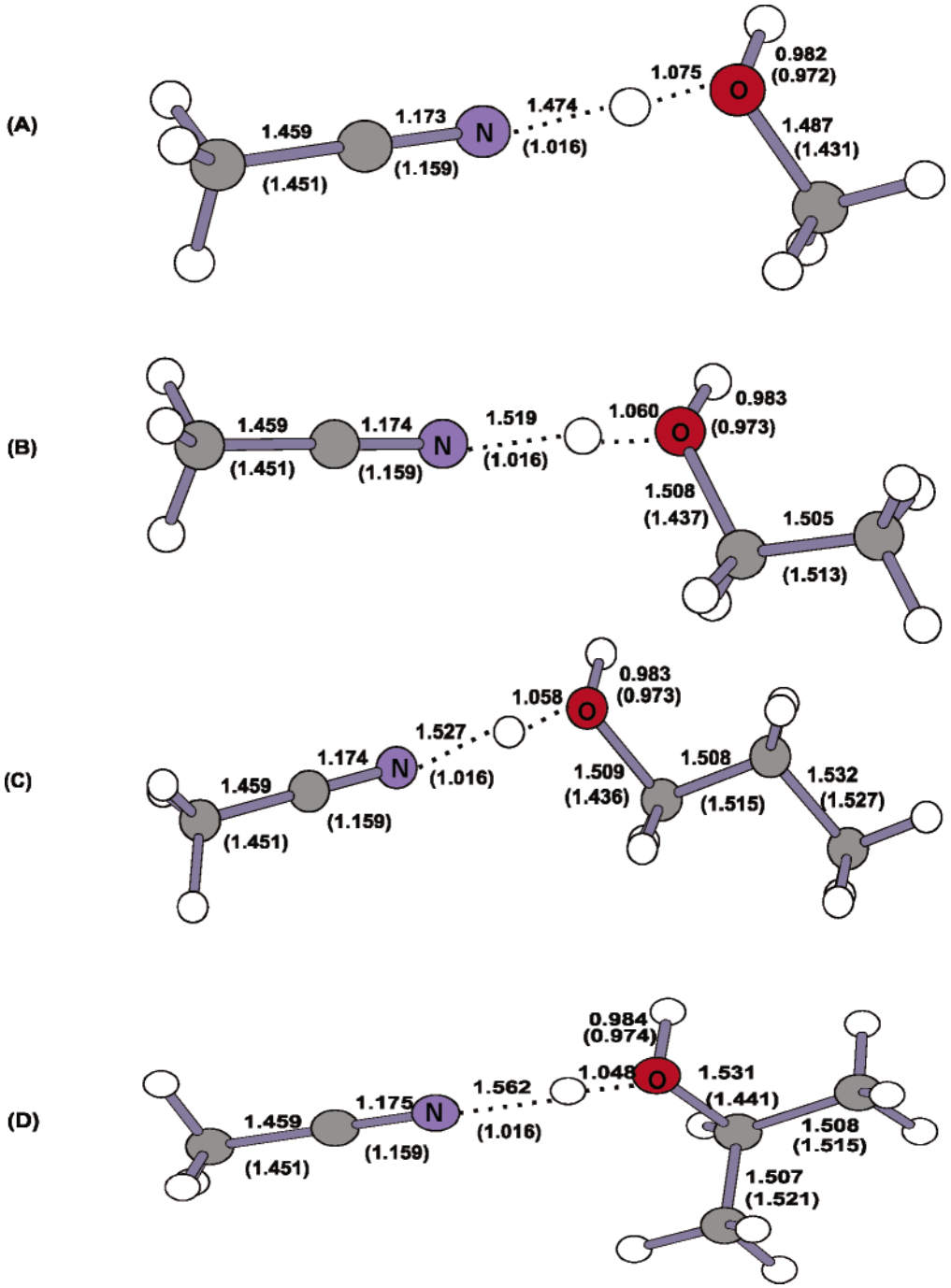

Figure 1. Selected optimized geometric parameters for the four proton-bound complexes obtained at the MP2/6-31+G(d) level of theory. Values corresponding to the free products are in parentheses.

CH_2OH and $CH_3CNH^+ + (CH_3)_2CHOH$. Incorrect product vibrational frequencies and moments of inertia were listed in Table 1, and incorrect product geometries are quoted in parentheses in Figure 3 for these two systems. The corrected Table (Table 1) and Figure (Figure 1) are shown below. As is evident from the new figure, the same trends in C−O bond length and ∠HOC and ∠OCC angles are observed across all four proton-bound pairs (page 9730, column 2, lines 16−21). The corrections are typographical only and do not alter any of the calculated α or $\Delta S^{\ddagger}$ values, which employed the correct values. The conclusions remain as they are.

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