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SUPPLEMENTARY MATERIAL TO

Understanding the isomerization kinetics in the gas phase of a triazole-3-thione derivative: A theoretical approach

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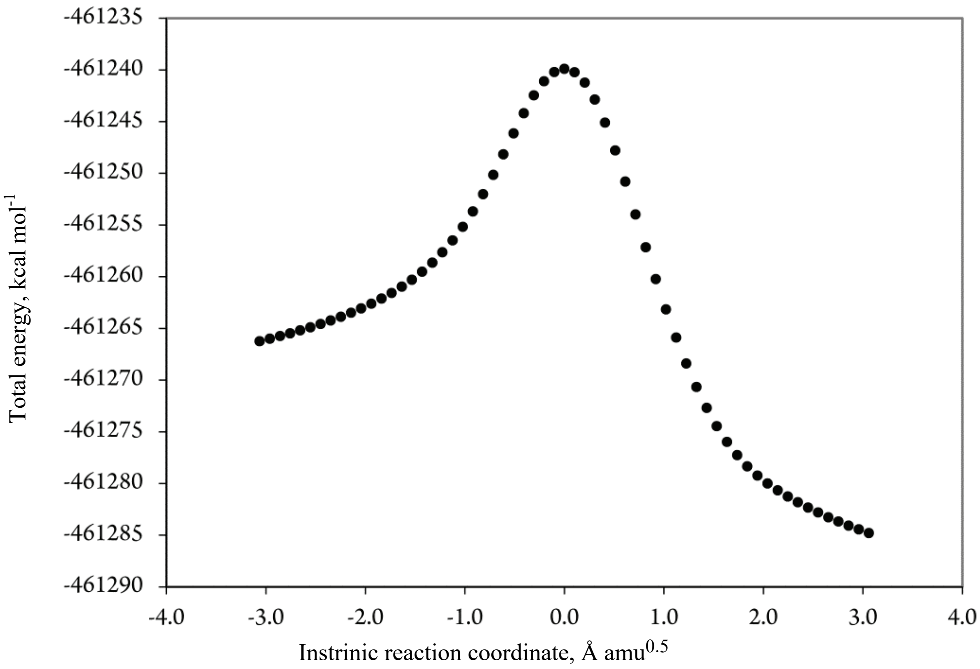

Fig. S-1. IRC reaction profile for the isomerization reactions at the B3LYP/6-31G** level of theory.

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TABLE S-I. Unscaled harmonic vibrational frequencies and rotational moments of inertia calculated at the M06-2*x*/aug-cc-pVTZ level of theory for the isomerization reaction

Parameter	Isomer **1**	Isomer **2**	TS
Frequency cm^{-1}	55.2449, 130.2018, 192.4864, 227.3407, 242.7213, 278.2738, 325.9454, 482.2948, 542.4114, 551.9155, 682.4364, 701.9709, 718.2042, 773.3892, 977.0001, 1008.7240, 1065.4283, 1094.7484, 1140.5642, 1242.9855, 1289.2294, 1360.1567, 1372.0035, 1419.0202, 1468.4242, 1471.7313, 1512.4162, 1529.3193, 1675.5690, 1711.8682, 3063.4133, 3129.4914, 3167.0760, 3480.1831, 3542.2318, 3674.0244	48.4272, 130.4943, 191.9482, 219.6245, 262.1253, 262.7366, 320.2943, 327.2367, 455.1776, 506.0384, 682.0307, 703.7806, 712.6314, 746.0717, 893.6517, 903.3288, 1017.4332, 1035.6807, 1066.0867, 1094.2074, 1283.8054, 1339.3676, 1388.1442, 1410.7638, 1467.5036, 1474.7717, 1504.7300, 1545.4519, 1621.5350, 1689.6031, 2764.3374, 3059.9085, 3122.5179, 3164.3833, 3490.7693, 3577.9944	1639.5988i, 114.9908, 163.9318, 213.0267, 231.3504, 232.7676, 270.9506, 303.4780, 516.6405, 553.1330, 661.6608, 694.3645, 715.3674, 776.0212, 834.0766, 925.3748, 1028.8116, 1058.8051, 1076.5138, 1118.2048, 1291.7369, 1347.6654, 1393.4790, 1421.5809, 1481.5258, 1484.7025, 1504.9572, 1531.5572, 1634.3479, 1688.8733, 1783.7447, 3080.1349, 3144.4173, 3178.9315, 3492.1824, 3573.6736
I_a, I_b, I_c amu Bohr^2	509.69582, 1305.95347, 1795.08451	508.37502, 1322.54876, 1809.95100	498.34025, 1357.61157, 1835.08234

TABLE S-II. Unscaled harmonic vibrational frequencies and rotational moments of inertia calculated by the CBS-QB3 composite method for the isomerization reaction.

Parameter	Isomer **1**	Isomer **2**	TS
Frequency cm^{-1}	113.0072, 125.7471, 191.1023, 227.8474, 228.6209, 275.6369, 315.7505, 476.1230, 522.6864, 537.1115, 671.0696, 680.0331, 705.1430, 755.5083, 959.3587, 1001.9336, 1069.7548, 1075.5519, 1104.4466, 1220.0681, 1272.2126, 1330.3889, 1363.5075, 1418.8553, 1456.7670, 1473.1195, 1486.9856, 1499.6876, 1633.4028, 1712.1867, 3048.8329, 3103.1523, 3146.2706, 3452.0011, 3513.6357, 3672.1069	102.2564, 130.1217, 165.6836, 194.7097, 235.5641, 264.4359, 305.3353, 322.0429, 441.8617, 503.1562, 667.3470, 684.7839, 688.8315, 731.5168, 879.7810, 922.7832, 1008.1073, 1018.4884, 1046.7244, 1066.8692, 1260.7010, 1328.7766, 1351.5215, 1413.4393, 1432.5634, 1474.1733, 1476.4475, 1502.3931, 1579.0524, 1691.0588, 2690.2523, 3040.9304, 3091.7401, 3141.9804, 3478.3378, 3563.9799	1624.5666i, 92.2540, 116.2546, 205.4695, 232.2021, 248.5426, 266.3684, 289.4769, 504.1698, 546.1197, 645.2433, 671.9545, 698.8084, 759.0373, 821.1583, 907.9839, 1016.0032, 1033.9422, 1062.9438, 1065.1457, 1265.4215, 1343.1092, 1357.2672, 1414.7334, 1444.0185, 1473.2902, 1473.4526, 1491.7363, 1586.0496, 1695.0065, 1745.8091, 3042.6232, 3094.4524, 3144.1992, 3478.0734, 3558.1432
I_a, I_b, I_c amu Bohr^2	515.46105, 1323.36174, 1818.13739	514.23739, 1342.84370, 1835.98942	504.16943, 1374.23706, 1857.43095

TABLE S-III. Structural parameters for all stationary points involved in the isomerization reactions optimized at different levels of theory. (See Scheme 1 for atom labeling)

Parameter	B3LYP/aug-cc-pVTZ			M06-2*x*/aug-cc-pVTZ			CBS-QB3		
	Isomer **1**	TS	Isomer **2**	Isomer **1**	TS	Isomer **2**	Isomer **1**	TS	Isomer **2**
r (N_1–N_2) / Å	1.374	1.381	1.391	1.367	1.373	1.382	1.376	1.381	1.393
r (N_2–C_3) / Å	1.351	1.317	1.299	1.345	1.311	1.296	1.354	1.319	1.301
r (C_3–N_4) / Å	1.385	1.354	1.373	1.375	1.348	1.365	1.389	1.358	1.377
r (N_4–C_5) / Å	1.378	1.396	1.377	1.374	1.388	1.371	1.382	1.399	1.381
r (N_1–C_5) / Å	1.298	1.303	1.306	1.293	1.299	1.299	1.300	1.306	1.305
r (N_2–H_6) / Å	1.004	1.379	–	1.005	1.369	–	1.007	1.388	–
r (C_3–S_7) / Å	1.665	1.721	1.761	1.662	1.716	1.751	1.666	1.723	1.763
r (S_7–H_6) / Å	–	1.727	1.345	–	1.713	1.340	–	1.722	1.343
∠ H_6–N_2–C_3 / °	125.31	82.08	–	125.04	81.17	–	125.16	81.85	–
∠ N_2–C_3–S_7 / °	130.87	109.76	128.00	131.20	110.19	128.66	130.86	109.74	128.12
∠ C_3–S_7–H_6 / °	–	61.78	92.98	–	61.15	92.77	–	61.97	92.92
φ (H_6–N_2–C_3–S_7) / °	0.0	0.0	–	0.0	0.0	–	0.0	0.0	–
φ (H_6–N_2–C_3–N_4) / °	–180.0	180.0	–	–180.0	–180.0	–	179.98	–180.0	–
φ (N_2–C_3–S_7–H_6) / °	–	0.0	0.0	–	0.0	0.0	–	0.0	0.0
φ (N_1–N_2–C_3–S_7) / °	–180.0	–180.0	180.0	–180.0	180.0	–180.0	–180.0	180.0	–180.0