Supplementary Materials

The study of structural features of N- and O-derivatives of 4,5-dihydroxyimidazolidine-2-thione by NMR spectroscopy and quantum-chemical calculations

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Table S1. The comparison of geometric parameters of **1t** optimized molecular structure and experimental data [17].

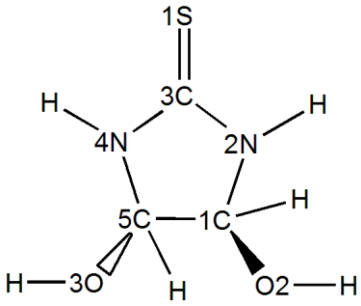
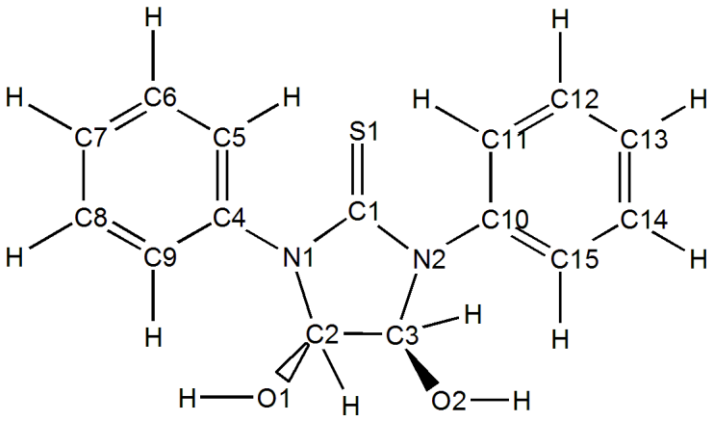
Parameter	Experimental data	Calculation data M062X/6-311+G(d,p)
		
Bond, Å		
1S-3C	1.6909	1.674
2N-3C	1.3421	1.355
2N-1C	1.4523	1.449
4N-3C	1.3453	1.355
4N-5C	1.4559	1.450
2O-1C	1.4045	1.400
3O-5C	1.4087	1.400
5C-1C	1.5440	1.548
Angle, °		
2N3C4N	109.0	107.23
2O1C5C3O	139.6	141.65

Table S2. The comparison of geometric parameters of **4t** optimized molecular structure and experimental data [18].

Parameter	Experimental data	Calculation data M062X/6-311+G(d,p)
		
Bond, Å		
S1—C1	1.669	1.672
O1—C2	1.427	1.401
O2—C3	1.416	1.397
N1—C1	1.357	1.365

N1—C4	1.444	1.428
N1—C2	1.459	1.460
N2—C1	1.373	1.360
N2—C10	1.433	1.427
N2—C3	1.454	1.457
C2—C3	1.526	1.534
C4—C9	1.374	1.391
C4—C5	1.396	1.393
C5—C6	1.394	1.390
C6—C7	1.368	1.393
C7—C8	1.387	1.392
C8—C9	1.394	1.392
C10—C15	1.390	1.392
C10—C11	1.393	1.391
C11—C12	1.389	1.392
C12—C13	1.386	1.392
C13—C14	1.384	1.393
C14—C15	1.384	1.390
Angle, °		
C1—N1—C4	126.4	125.31
C1—N1—C2	110.97	111.24
C4—N1—C2	122.5	120.15
C1—N2—C10	126.6	125.85
C1—N2—C3	111.1	112.11
C10—N2—C3	119.53	121.26
N1—C1—N2	108.0	107.57
N1—C1—S1	125.46	126.09
N2—C1—S1	126.6	126.33
O1—C2—N1	111.04	112.31
O1—C2—C3	110.76	108.15
N1—C2—C3	102.8	101.91
O2—C3—N2	112.5	112.44
O2—C3—C2	113.8	114.15
N2—C3—C2	101.37	101.64
C9—C4—C5	119.9	120.82
C9—C4—N1	119.9	119.00
C5—C4—N1	120.1	120.13
C6—C5—C4	119.6	119.42
C7—C6—C5	120.9	120.10
C6—C7—C8	119.0	120.14
C7—C8—C9	121.1	120.06
C4—C9—C8	119.5	119.47
C15—C10—C11	120.3	120.83
C15—C10—N2	120.0	120.30
C11—C10—N2	119.6	118.85
C12—C11—C10	119.4	119.51
C13—C12—C11	119.9	120.03
C14—C13—C12	120.7	120.09
C15—C14—C13	119.6	120.16
C14—C15—C10	120.1	119.39

Table S3. Cartesian coordinates of the optimized structures

Structure	Atom	X	Y	Z
1c	C	-1.3361	-0.7632	0.2480
	C	-1.2760	0.7885	0.2216
	C	0.8494	-0.0681	-0.1592
	H	-1.4312	-1.1363	1.2691
	H	-1.7892	1.2440	1.0657
	N	-0.0157	-1.0924	-0.2902
	H	0.3197	-2.0422	-0.3584
	N	0.1525	1.0113	0.2803
	H	0.5566	1.9344	0.2133
	S	2.4975	-0.1101	-0.4659
	O	-2.3807	-1.2893	-0.4887
	H	-2.4975	-0.7288	-1.2691
	O	-1.8260	1.2156	-1.0004
	H	-2.3025	2.0422	-0.8814
1t	C	-1.6024	0.6843	0.3620
	C	-1.6024	-0.6842	-0.3618
	C	0.5928	-0.0001	0.0001
	H	-2.2666	0.6706	1.2238
	H	-2.2666	-0.6703	-1.2237
	N	-0.2106	0.7885	0.7532
	H	0.1622	1.5529	1.2964
	N	-0.2107	-0.7885	-0.7532
	H	0.1622	-1.5527	-1.2964
	S	2.2666	0.0000	0.0000
	O	-2.0242	1.7451	-0.4489
	H	-1.4509	1.8078	-1.2227
	O	-2.0242	-1.7451	0.4488
	H	-1.4509	-1.8078	1.2227
2c	C	-1.3307	-0.5712	0.2162
	C	-1.0828	0.9406	0.0417
	C	0.9020	-0.1985	-0.2729
	H	-1.4397	-0.8366	1.2718
	H	-1.5212	1.5402	0.8387
	N	-0.0797	-1.1241	-0.3060
	N	0.3621	1.0050	0.0720
	S	2.5286	-0.4830	-0.5846
	O	-2.4533	-1.0347	-0.4477
	H	-2.5286	-0.5326	-1.2718
	O	-1.5936	1.3219	-1.2164
	H	-1.9709	2.2052	-1.1715
	C	0.1443	-2.5561	-0.3235
	H	0.8536	-2.8022	-1.1113
	H	0.5359	-2.9077	0.6358
	H	-0.8089	-3.0395	-0.5312

	C	1.0443	2.2741	-0.1061
	H	2.0466	2.2045	0.3109
	H	1.1123	2.5473	-1.1626
	H	0.4841	3.0395	0.4309
2t	C	1.5960	-0.7695	0.0103
	C	1.5960	0.7694	-0.0103
	C	-0.5856	-0.0000	-0.0001
	H	2.2630	-1.1592	0.7788
	H	2.2630	1.1591	-0.7788
	N	0.2086	-1.0547	0.3216
	N	0.2085	1.0545	-0.3216
	S	-2.2630	-0.0001	0.0000
	O	2.0089	-1.3496	-1.1990
	H	1.4551	-1.0225	-1.9187
	O	2.0089	1.3494	1.1990
	H	1.4550	1.0223	1.9187
	C	-0.2654	-2.4150	0.4992
	H	-1.1240	-2.4150	1.1680
	H	-0.5535	-2.8648	-0.4542
	H	0.5406	-2.9975	0.9441
	C	-0.2655	2.4148	-0.4991
	H	-1.1241	2.4148	-1.1679
	H	-0.5536	2.8645	0.4543
	H	0.5405	2.9975	-0.9439
3c	C	-1.0693	0.8733	-0.0213
	C	0.4546	1.0724	-0.2105
	C	-0.1200	-1.0927	-0.8034
	H	-1.3302	0.8027	1.0379
	H	0.9341	1.5018	0.6692
	N	-1.2832	-0.4155	-0.6779
	N	0.9061	-0.2748	-0.4564
	S	0.0385	-2.6946	-1.3034
	O	-1.8329	1.8948	-0.5638
	H	-1.4081	2.1638	-1.3907
	O	0.6938	1.8731	-1.3488
	H	1.1220	2.6946	-1.0895
	C	-2.6075	-1.0214	-0.7047
	H	-2.6197	-1.7443	-1.5197
	H	-3.3089	-0.2228	-0.9515
	C	2.3234	-0.5865	-0.5884
	H	2.4363	-1.3100	-1.3955
	H	2.8244	0.3345	-0.8933
	C	2.9070	-1.1263	0.7114
	H	2.7895	-0.4013	1.5197
	H	2.4010	-2.0505	0.9957
	H	3.9713	-1.3345	0.5878

	C	-2.9753	-1.6872	0.6175
	H	-3.9713	-2.1277	0.5463
	H	-2.2614	-2.4782	0.8537
	H	-2.9834	-0.9645	1.4360
3t	C	-0.7070	-1.6321	-0.3095
	C	0.7069	-1.6321	0.3095
	C	0.0000	0.5596	-0.0000
	H	-1.3879	-2.2441	0.2836
	H	1.3879	-2.2441	-0.2836
	N	-1.0688	-0.2306	-0.2615
	N	1.0688	-0.2306	0.2615
	S	0.0000	2.2441	-0.0000
	O	-0.7579	-2.1490	-1.6127
	H	-0.2115	-1.6037	-2.1924
	O	0.7579	-2.1490	1.6127
	H	0.2115	-1.6037	2.1924
	C	-2.4325	0.2230	-0.4985
	H	-2.3803	1.1792	-1.0193
	H	-2.8913	-0.5023	-1.1733
	C	2.4325	0.2230	0.4984
	H	2.3803	1.1792	1.0193
	H	2.8913	-0.5023	1.1733
	C	3.2244	0.3512	-0.7967
	H	4.2439	0.6769	-0.5827
	H	3.2733	-0.6064	-1.3196
	H	2.7550	1.0853	-1.4542
	C	-3.2244	0.3512	0.7967
	H	-4.2439	0.6769	0.5826
	H	-3.2733	-0.6064	1.3196
	H	-2.7550	1.0853	1.4542
4c	C	-0.7871	1.1546	0.7546
	C	0.7413	1.2162	0.5613
	C	-0.0129	-0.9149	-0.0131
	H	-1.0540	1.0826	1.8119
	H	1.2641	1.6343	1.4206
	N	-1.1077	-0.1210	0.0885
	N	1.0742	-0.1898	0.3861
	S	0.0100	-2.5116	-0.5161
	O	-1.4621	2.2358	0.2247
	H	-0.9949	2.5116	-0.5769
	O	0.9902	1.9617	-0.6023
	H	1.8737	2.3422	-0.5760
	C	-2.4573	-0.5835	0.0376
	C	-2.9564	-1.3951	1.0533
	C	-3.2712	-0.1768	-1.0131
	C	-4.2816	-1.8116	1.0063

	H	-2.3043	-1.7000	1.8640
	C	-4.5991	-0.5927	-1.0522
	H	-2.8582	0.4572	-1.7883
	C	-5.1030	-1.4107	-0.0457
	H	-4.6735	-2.4483	1.7903
	H	-5.2367	-0.2794	-1.8700
	H	-6.1357	-1.7369	-0.0792
	C	2.4329	-0.5827	0.1807
	C	3.2200	-0.8793	1.2878
	C	2.9669	-0.6187	-1.1050
	C	4.5565	-1.2229	1.1066
	H	2.7801	-0.8425	2.2777
	C	4.3014	-0.9667	-1.2799
	H	2.3331	-0.3823	-1.9518
	C	5.0959	-1.2681	-0.1755
	H	5.1725	-1.4590	1.9658
	H	4.7217	-1.0007	-2.2777
	H	6.1357	-1.5381	-0.3161
4t	C	-0.7624	1.6030	0.0992
	C	0.7511	1.6213	-0.1468
	C	0.0023	-0.5934	-0.0677
	H	-1.2949	2.2659	-0.5856
	H	1.2549	2.2392	0.5949
	N	-1.0960	0.2096	-0.1787
	N	1.0937	0.2135	0.0220
	S	0.0030	-2.2659	-0.0578
	O	-0.9911	1.9480	1.4373
	H	-1.9393	2.0344	1.5890
	O	1.1204	2.1134	-1.4013
	H	0.7008	1.5860	-2.0926
	C	-2.4516	-0.2316	-0.1047
	C	-2.9498	-0.7640	1.0821
	C	-3.2757	-0.0667	-1.2128
	C	-4.2853	-1.1436	1.1528
	H	-2.2870	-0.8834	1.9313
	C	-4.6132	-0.4425	-1.1333
	H	-2.8641	0.3495	-2.1252
	C	-5.1168	-0.9823	0.0468
	H	-4.6775	-1.5608	2.0724
	H	-5.2592	-0.3175	-1.9938
	H	-6.1577	-1.2770	0.1055
	C	2.4530	-0.2194	0.0512
	C	3.2029	0.0014	1.2012
	C	3.0240	-0.8159	-1.0690
	C	4.5408	-0.3810	1.2310
	H	2.7361	0.4650	2.0629

	C	4.3584	-1.2040	-1.0298
	H	2.4199	-0.9778	-1.9541
	C	5.1172	-0.9860	0.1181
	H	5.1278	-0.2104	2.1252
	H	4.8073	-1.6719	-1.8976
	H	6.1577	-1.2871	0.1436
6c	C	-0.5764	-1.1467	-0.5574
	C	0.9659	-1.1981	-0.4088
	C	0.2579	1.0102	-0.1873
	H	-0.8860	-1.3531	-1.5835
	H	1.4466	-1.7470	-1.2179
	N	-0.8594	0.2492	-0.2238
	N	1.3338	0.1978	-0.4268
	S	0.3213	2.6633	0.0581
	O	-1.2468	-2.0464	0.2537
	H	-0.8473	-2.0120	1.1339
	O	1.3371	-1.7412	0.8443
	H	1.5957	-2.6633	0.7370
	C	2.7038	0.5724	-0.1428
	H	2.8777	1.5744	-0.5267
	H	3.3390	-0.1443	-0.6699
	O	2.9907	0.5966	1.2339
	H	2.7868	-0.2797	1.5835
	C	-2.2001	0.7334	-0.0666
	H	-2.2598	1.7410	-0.4810
	H	-2.8592	0.0576	-0.6178
	O	-2.5181	0.7328	1.3126
	H	-3.3390	1.2205	1.4349
6t/6a	C	0.6684	-1.3436	-0.0443
	C	-0.8355	-1.2803	0.2481
	C	0.0106	0.8734	0.0631
	H	0.9078	-2.0380	-0.8530
	H	-1.0898	-1.9014	1.1093
	N	0.9467	0.0215	-0.4472
	N	-1.0160	0.1233	0.5473
	S	0.1298	2.5395	0.1091
	O	1.3232	-1.6897	1.1523
	H	2.2240	-1.3401	1.1219
	O	-1.6436	-1.5884	-0.8658
	H	-1.7950	-2.5395	-0.9018
	C	2.2814	0.4218	-0.8232
	H	2.2199	1.3873	-1.3231
	H	2.6782	-0.3308	-1.5025
	C	-2.3343	0.6356	0.8523
	H	-2.8148	-0.0997	1.5025
	H	-2.2279	1.5835	1.3746

	O	-3.0982	0.8787	-0.3030
	H	-3.1533	0.0477	-0.7909
	O	3.1533	0.4628	0.2888
	H	2.9443	1.2497	0.8071
6b	C	0.5605	1.3970	-0.1504
	C	-0.9568	1.1411	-0.1607
	C	0.1486	-0.8700	-0.4709
	H	0.8694	1.9368	0.7469
	H	-1.4557	1.8245	-0.8507
	N	1.0900	0.0428	-0.1442
	N	-1.0446	-0.2276	-0.6161
	S	0.4238	-2.5133	-0.6626
	O	0.8944	2.0982	-1.3181
	H	1.7572	2.5133	-1.2181
	O	-1.5386	1.2008	1.1239
	H	-1.8020	2.1074	1.3181
	C	2.4886	-0.2937	0.0520
	H	3.0454	0.6396	0.1189
	H	2.8315	-0.8664	-0.8122
	C	-2.3300	-0.8935	-0.6491
	H	-3.0454	-0.1717	-1.0507
	H	-2.2601	-1.7543	-1.3096
	O	-2.7301	-1.3676	0.6125
	H	-2.7479	-0.6091	1.2093
	O	2.7072	-0.9995	1.2426
	H	2.3295	-1.8806	1.1211
6d	C	-0.7653	1.2935	0.0387
	C	0.7651	1.2936	-0.0387
	C	-0.0000	-0.8992	0.0000
	H	-1.1839	1.5960	-0.9274
	H	1.1837	1.5962	0.9275
	N	-1.0608	-0.1135	0.2998
	N	1.0608	-0.1134	-0.2997
	S	0.0002	-2.5821	0.0000
	O	-1.2041	2.1288	1.0637
	H	-2.0094	2.5817	0.7972
	O	1.2038	2.1289	-1.0637
	H	2.0090	2.5821	-0.7971
	C	-2.4143	-0.6204	0.3739
	H	-3.0426	0.1792	0.7625
	H	-2.4182	-1.4612	1.0683
	C	2.4144	-0.6201	-0.3739
	H	2.4184	-1.4609	-1.0684
	H	3.0426	0.1796	-0.7623
	O	2.9263	-0.9894	0.8812
	H	2.4828	-1.8051	1.1456

	O	-2.9263	-0.9896	-0.8812
	H	-2.4826	-1.8053	-1.1456
9c	C	0.6730	-0.8902	0.3447
	C	0.3895	0.6240	0.4620
	C	-1.5745	-0.5036	-0.0922
	H	0.7428	-1.3353	1.3464
	H	0.7763	1.0493	1.3915
	N	-0.5518	-1.3622	-0.3110
	H	-0.7637	-2.3442	-0.4153
	N	-1.0656	0.6168	0.4677
	H	-1.6353	1.4416	0.5818
	S	-3.1918	-0.7877	-0.4305
	O	1.8266	-1.1310	-0.3732
	O	0.9248	1.2866	-0.6401
	C	0.8233	2.7002	-0.5484
	H	1.2656	3.0593	0.3865
	H	1.3742	3.1112	-1.3915
	H	-0.2179	3.0305	-0.6096
	C	2.2144	-2.4987	-0.3640
	H	1.5084	-3.1112	-0.9323
	H	3.1918	-2.5523	-0.8378
	H	2.2831	-2.8743	0.6618
9t	C	-1.3806	0.6853	0.3462
	C	-1.3803	-0.6847	-0.3463
	C	0.8173	0.0008	-0.0001
	H	-2.0186	0.6880	1.2337
	H	-2.0184	-0.6877	-1.2338
	N	0.0181	0.8236	0.7121
	N	0.0184	-0.8223	-0.7124
	S	2.4956	0.0011	-0.0001
	O	-1.8007	1.6395	-0.5839
	O	-1.7998	-1.6391	0.5838
	C	-1.8645	-2.9551	0.0528
	H	-2.4949	-2.9786	-0.8419
	H	-2.3034	-3.5852	0.8230
	C	-1.8657	2.9555	-0.0530
	H	-2.4956	2.9788	0.8420
	H	-2.3054	3.5852	-0.8231
	H	0.3940	1.5243	1.3311
	H	0.3946	-1.5231	-1.3311
	H	-0.8684	3.3324	0.1902
	H	-0.8672	-3.3316	-0.1912
10t	C	-0.7328	-0.9763	0.2403
	C	0.7327	-0.9762	-0.2403
	C	-0.0002	1.2181	-0.0000
	H	-0.8526	-1.6280	1.1090

	H	0.8526	-1.6279	-1.1090
	N	-0.9109	0.4217	0.6000
	N	0.9106	0.4219	-0.6000
	S	-0.0003	2.8974	-0.0000
	O	-1.5575	-1.3752	-0.8142
	O	1.5574	-1.3750	0.8141
	C	2.7802	-2.0044	0.4217
	H	2.5456	-2.8972	-0.1684
	H	3.2383	-2.3255	1.3566
	C	-2.7802	-2.0046	-0.4217
	H	-2.5455	-2.8974	0.1685
	H	-3.2383	-2.3257	-1.3566
	C	3.7145	-1.0840	-0.3444
	H	3.8918	-0.1613	0.2124
	H	3.3195	-0.8378	-1.3335
	C	-3.7145	-1.0842	0.3444
	H	-3.8919	-0.1617	-0.2124
	H	-3.3194	-0.8379	1.3335
	H	-1.7638	0.8055	0.9776
	H	1.7634	0.8058	-0.9776
	H	-4.6727	-1.5845	0.4959
	H	4.6727	-1.5841	-0.4957
11t	C	-0.7447	-0.9785	0.2001
	C	0.7446	-0.9784	-0.2002
	C	-0.0002	1.2151	-0.0001
	H	-0.9146	-1.6342	1.0572
	H	0.9146	-1.6341	-1.0575
	N	-0.9385	0.4183	0.5557
	N	0.9381	0.4185	-0.5557
	S	-0.0003	2.8945	-0.0001
	O	-1.5112	-1.3694	-0.9006
	O	1.5111	-1.3692	0.9005
	C	2.7541	-1.9965	0.5817
	H	2.5590	-2.8944	-0.0184
	H	3.1630	-2.3135	1.5423
	C	-2.7542	-1.9966	-0.5817
	H	-2.5590	-2.8945	0.0182
	H	-3.1631	-2.3137	-1.5423
	C	3.7410	-1.0867	-0.1352
	H	3.8345	-0.1506	0.4238
	H	3.3646	-0.8430	-1.1347
	C	-3.7410	-1.0868	0.1350
	H	-3.8347	-0.1508	-0.4240
	H	-3.3646	-0.8430	1.1345
	H	-1.8068	0.8015	0.8971
	H	1.8064	0.8017	-0.8972

	C	-5.1025	-1.7660	0.2673
	H	-5.8040	-1.1324	0.8111
	H	-5.5287	-1.9762	-0.7165
	H	-5.0159	-2.7124	0.8069
	C	5.1025	-1.7658	-0.2673
	H	5.8040	-1.1323	-0.8110
	H	5.5286	-1.9759	0.7167
	H	5.0160	-2.7123	-0.8067
12t	C	0.7568	-0.9882	-0.1495
	C	-0.7568	-0.9882	0.1494
	C	0.0000	1.2070	-0.0001
	H	0.9828	-1.6362	-0.9997
	H	-0.9828	-1.6362	0.9996
	N	0.9786	0.4107	-0.4803
	N	-0.9786	0.4107	0.4802
	S	-0.0001	2.8868	-0.0001
	O	1.4458	-1.3935	0.9960
	O	-1.4457	-1.3936	-0.9961
	C	-2.7119	-2.0096	-0.7542
	H	-2.5664	-2.8868	-0.1113
	H	-3.0459	-2.3578	-1.7325
	C	2.7120	-2.0095	0.7541
	H	2.5664	-2.8867	0.1112
	H	3.0460	-2.3577	1.7325
	C	-3.7474	-1.0742	-0.1482
	H	-3.7890	-0.1532	-0.7401
	H	-3.4557	-0.8013	0.8734
	C	-5.1280	-1.7273	-0.1028
	H	-5.4350	-1.9861	-1.1213
	H	-5.0652	-2.6680	0.4542
	C	-6.1748	-0.8195	0.5375
	H	-6.2663	0.1180	-0.0169
	H	-7.1559	-1.2973	0.5568
	H	-5.8990	-0.5743	1.5664
	C	3.7474	-1.0741	0.1480
	H	3.7891	-0.1531	0.7399
	H	3.4557	-0.8013	-0.8736
	C	5.1280	-1.7273	0.1026
	H	5.4351	-1.9861	1.1210
	H	5.0652	-2.6680	-0.4545
	C	6.1748	-0.8195	-0.5379
	H	6.2664	0.1180	0.0165
	H	7.1559	-1.2973	-0.5573
	H	5.8989	-0.5742	-1.5667
	H	1.8669	0.7944	-0.7643
	H	-1.8669	0.7943	0.7642