ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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SUPPLEMENTARY MATERIALS TO: SYNTHESIS, CRYSTAL STRUCTURE, AND A DFT STUDY OF *TERT*-BUTYL-5-(4,4,5,5-TETRAMETHYL-1,3,2-DIOXABOROLAN-2-YL)-1*H*-INDAZOLE-1-CARBOXYLATE

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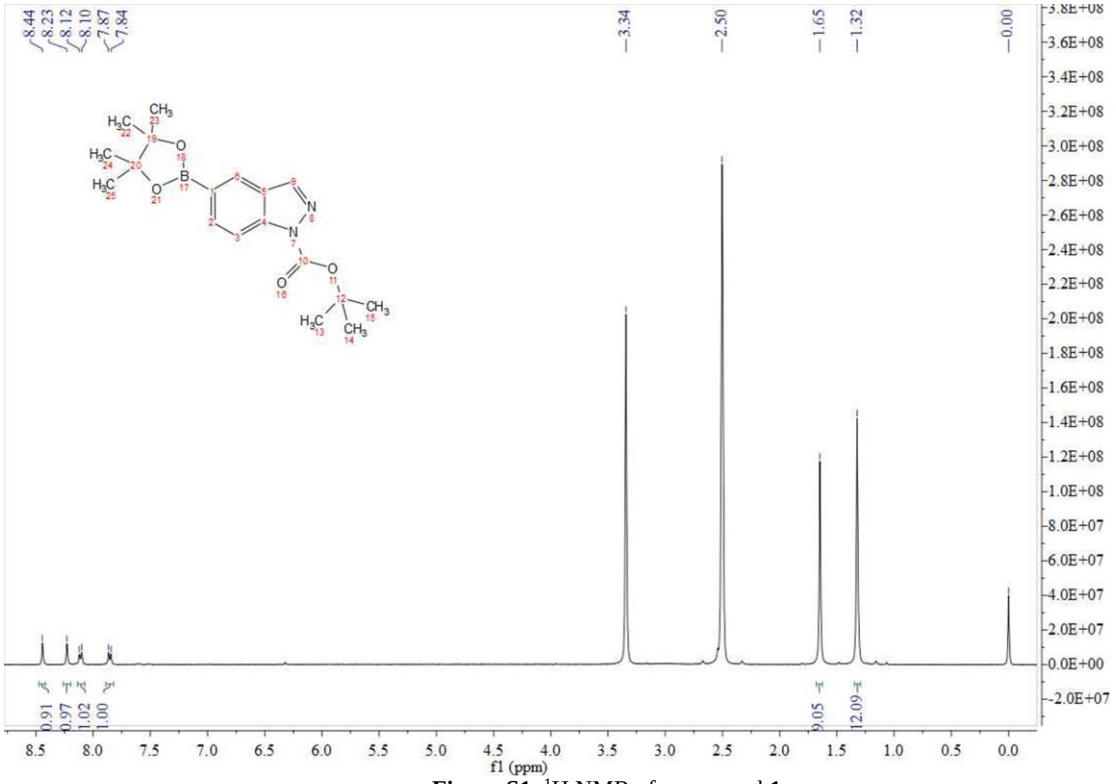


Figure S1. [1]H NMR of compound **1**.

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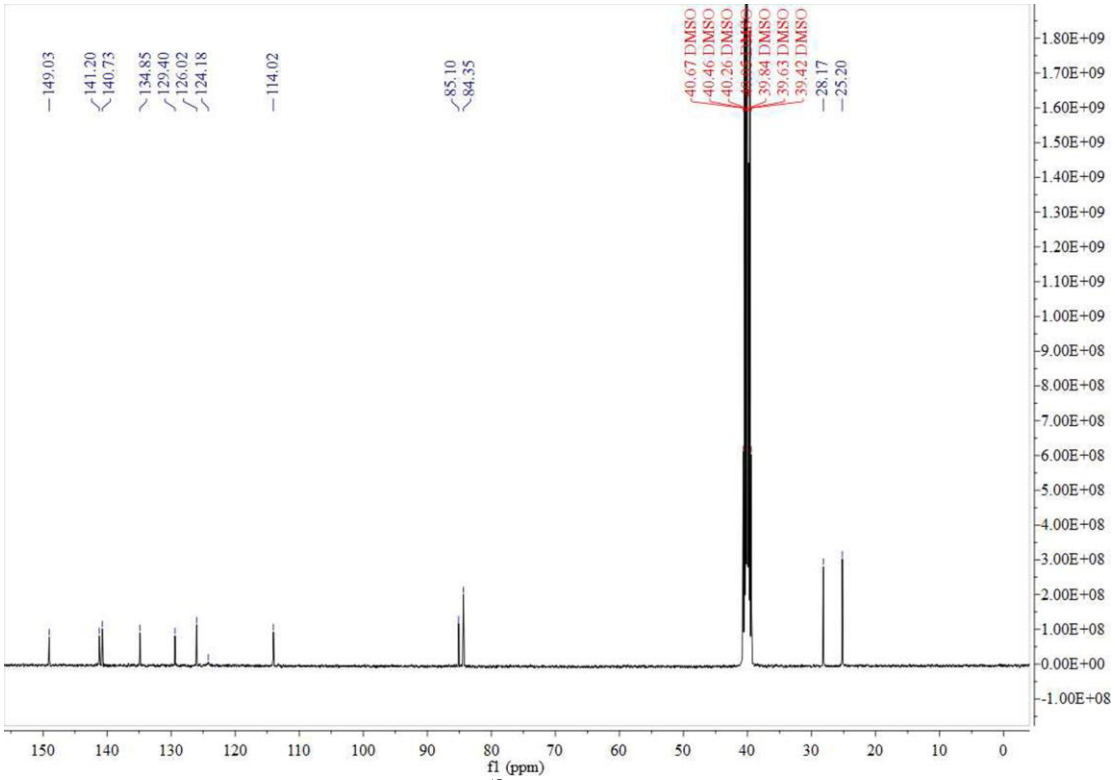


Figure S2. ^{13}C NMR of compound **1**.

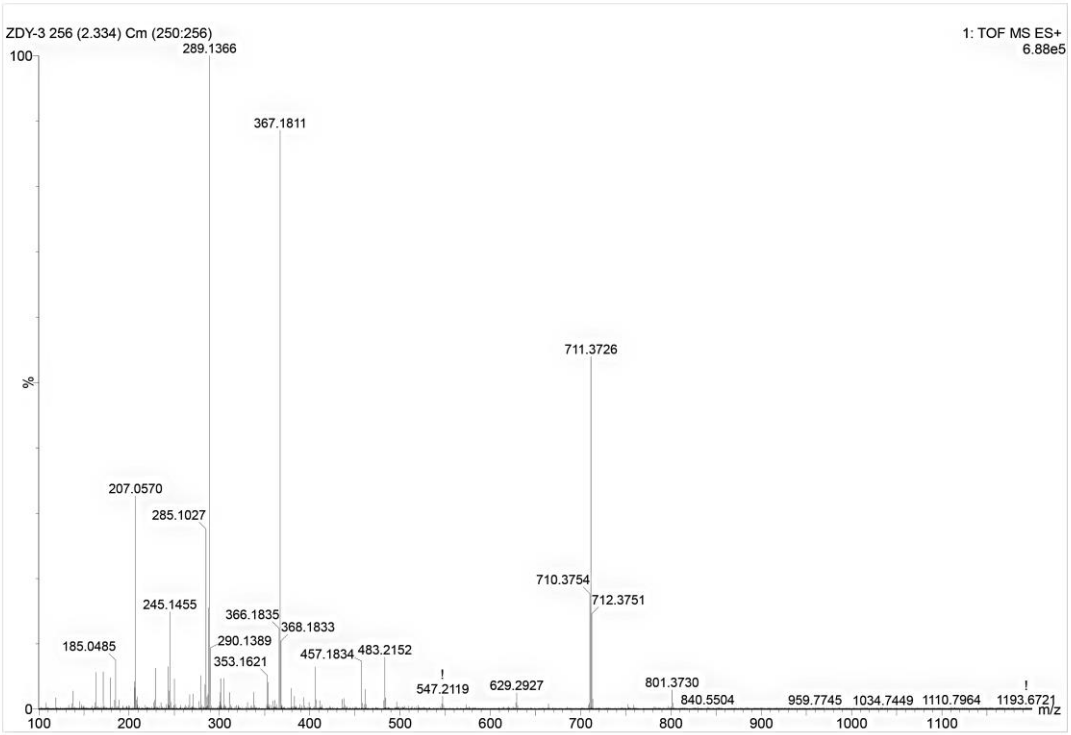


Figure S3. MS of compound **1**.

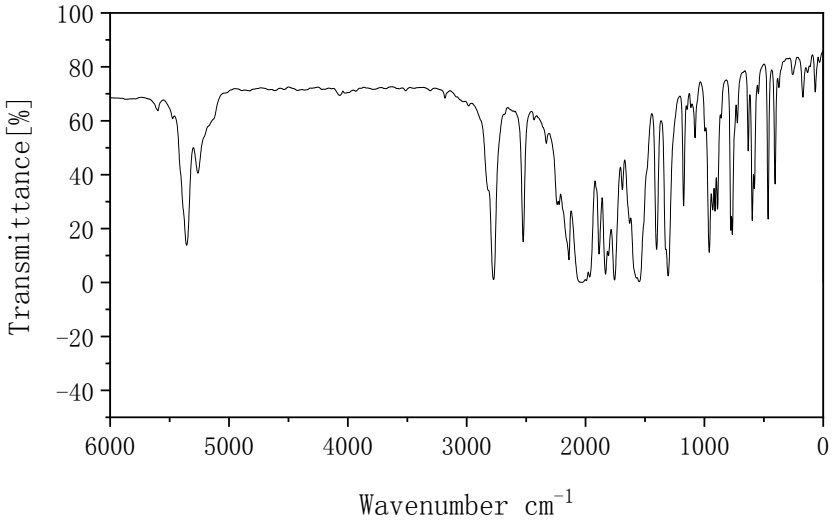


Figure S4. IR spectrum of compound **1**.

Table S1. Crystallographic characteristics, the X-ray data collection and structure-refinement parameters for compound **1**.

Compound	1
Empirical formula	$C_{18}H_{25}BN_2O_4$
Formula weight	344.21
Temperature/K	170.0
Crystal system	orthorhombic
Space group	Pbca
a/Å	8.7892(3)
b/Å	18.9939(7)
c/Å	22.6795(8)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3786.1(2)
Z	8
ρ_{calc}g/cm^3	1.208
μ/mm^{-1}	0.084
F(000)	1472.0
Crystal size/mm^3	0.19 × 0.13 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.288 to 52.77
Index ranges	-10 ≤ h ≤ 10, -23 ≤ k ≤ 23, -27 ≤ l ≤ 28
Reflections collected	22302
Independent reflections	3865 [R_{int} = 0.0748, R_{sigma} = 0.0508]
Data/restraints/parameters	3865/0/233
Goodness-of-fit on F^2	1.064
Final R indexes [$I>=2\sigma(I)$]	R_1 = 0.0492, wR_2 = 0.0974
Final R indexes [all data]	R_1 = 0.0965, wR_2 = 0.1203
Largest diff. peak/hole / e Å^{-3}	0.16/-0.17

Table S2. Bond distances, bond angles and torsion angles for compound **1** and conformer**1**.

Bond distance (Å)	**Exp.[a]**	**Calcd.[b]**	**Difference**
O(2)-C(2)	1.462	1.459	-0.003
O(2)-B(1)	1.336	1.374	0.038
O(1)-C(1)	1.466	1.458	-0.008
O(1)-B(1)	1.363	1.374	0.011
O(4)-C(14)	1.318	1.325	0.007
O(4)-C(15)	1.494	1.486	-0.008
O(3)-C(14)	1.202	1.210	0.008
N(1)-N(2)	1.392	1.380	-0.012
Bond distance (Å)	**Exp.[a]**	**Calcd.[b]**	**Difference**
N(1)-C(14)	1.404	1.408	0.004
N(1)-C(11)	1.389	1.392	0.003
N(2)-C(13)	1.309	1.306	-0.003
C(12)-C(7)	1.396	1.399	0.003
C(12)-C(11)	1.396	1.411	0.015
C(12)-C(13)	1.428	1.435	0.007
C(7)-C(8)	1.384	1.395	0.011
C(11)-C(10)	1.397	1.400	0.003
C(8)-C(9)	1.415	1.419	0.004
C(8)-B(1)	1.550	1.550	0.000
C(9)-C(10)	1.373	1.386	0.013
C(1)-C(5)	1.551	1.580	0.029
C(1)-C(2)	1.512	1.525	0.013
C(1)-C(3)	1.517	1.533	0.016
C(5)-C(4)	1.511	1.525	0.014
C(5)-C(6)	1.514	1.530	0.016
C(15)-C(17)	1.498	1.530	0.032
C(15)-C(16)	1.507	1.528	0.021
C(15)-C(18)	1.505	1.486	-0.019
Bond angle (°)	**Exp.[a]**	**Calcd.[b]**	**Difference**
B(1)-O(2)-C(5)	106.95	107.88	0.930
B(1)-O(1)-C(1)	107.11	107.95	0.840
C(14)-O(4)-C(15)	120.03	121.38	1.350
N(2)-N(1)-C(14)	121.96	122.44	0.480
C(11)-N(1)-N(2)	111.37	111.39	0.020
C(11)-N(1)-C(14)	126.64	126.18	-0.460
C(13)-N(2)-N(1)	105.00	106.15	1.150
C(7)-C(12)-C(11)	120.16	120.32	0.160

C(7)-C(12)-C(13)	135.03	135.10	0.070
C(11)-C(12)-C(13)	104.81	104.58	-0.230
C(8)-C(7)-C(12)	119.54	119.19	-0.350
O(4)-C(14)-N(1)	110.72	110.99	0.270
O(3)-C(14)-O(4)	128.58	127.86	-0.720
O(3)-C(14)-N(1)	120.70	121.15	0.450
N(1)-C(11)-C(12)	105.99	105.65	-0.340
N(1)-C(11)-C(10)	132.18	132.65	0.470
C(12)-C(11)-C(10)	121.81	121.70	-0.110
C(7)-C(8)-C(9)	118.44	118.96	0.520
C(7)-C(8)-B(1)	120.37	120.57	0.200
Bond angle (°)	**Exp.[a]**	**Calcd.[b]**	**Difference**
C(9)-C(8)-B(1)	121.16	120.45	-0.71
N(2)-C(13)-C(12)	112.82	112.23	-0.59
C(10)-C(9)-C(8)	123.52	123.1	-0.42
C(9)-C(10)-C(11)	116.52	116.73	0.21
O(1)-C(1)-C(5)	102.46	102.16	-0.30
O(1)-C(1)-C(2)	108.34	108.45	0.11
O(1)-C(1)-C(3)	106.29	106.67	0.38
C(2)-C(1)-C(5)	115.13	115.20	0.07
C(2)-C(1)-C(3)	110.29	110.14	-0.15
C(3)-C(1)-C(5)	113.54	113.46	-0.08
O(2)-C(5)-C(1)	102.64	102.15	-0.49
O(2)-C(5)-C(4)	106.34	106.61	0.27
O(2)-C(5)-C(6)	108.70	108.48	-0.22
C(4)-C(5)-C(1)	113.86	113.47	-0.39
C(4)-C(5)-C(6)	110.1	110.18	0.08
C(6)-C(5)-C(1)	114.50	115.18	0.68
O(4)-C(15)-C(17)	110.01	109.85	-0.16
O(4)-C(15)-C(16)	109.88	109.76	-0.12
O(4)-C(15)-C(18)	101.46	102.02	0.56
C(17)-C(15)-C(16)	112.46	112.69	0.23
C(17)-C(15)-C(18)	111.6	110.96	-0.64
C(18)-C(15)-C(16)	110.9	111.03	0.13
O(2)-B(1)-C(8)	122.93	123.71	0.78
O(2)-B(1)-O(2)	113.55	112.69	-0.86
O(1)-B(1)-C(8)	123.5	123.60	0.10
Torsion angle (°)	**Exp.[a]**	**Calcd.[b]**	**Difference**
B(1)-O(2)-C(5)-C(1)	-22.5(2)	-21.89	0.610

B(1)-O(2)-C(5)-C(4)	97.4(2)	97.41	0.010
B(1)-O(2)-C(5)-C(6)	-144.1(2)	-143.95	0.150
C(5)-O(2)-B(1)-O(1)	9.9(2)	9.31	-0.590
C(5)-O(2)-B(1)-O(8)	-170.6(2)	-170.64	-0.040
B(1)-O(1)-C(1)-C(5)	-21.6(2)	-21.81	-0.210
B(1)-O(1)-C(1)-C(2)	-143.7(2)	-143.89	-0.190
B(1)-O(1)-C(1)-C(3)	97.8(2)	97.50	-0.300
C(1)-O(1)-B(1)-O(2)	8.4(2)	9.16	0.760
C(1)-O(1)-B(1)-C(8)	-171.1(2)	-170.89	0.210
C(15)-O(4)-C(14)-O(3)	0.5(3)	0.20	-0.300
C(15)-O(4)-C(14)-N(1)	-178.8(1)	-179.86	-1.060
C(14)-O(4)-C(15)-C(17)	-61.4(2)	-62.01	-0.610
Torsion angle (°)	**Exp.[a]**	**Calcd.[b]**	**Difference**
C(14)-O(4)-C(15)-C(16)	62.9(2)	62.42	-0.480
C(14)-O(4)-C(15)-C(18)	-179.7(2)	-179.78	-0.080
C(14)-N(1)-N(2)-C(13)	178.2(2)	180.00	1.800
C(11)-N(1)-N(2)-C(13)	-0.0(2)	-0.03	-0.030
N(2)-N(1)-C(14)-O(4)	0.6(2)	0.72	0.120
N(2)-N(1)-C(14)-O(3)	-178.7(2)	-179.33	-0.630
C(11)-N(1)-C(14)-O(4)	178.6(2)	179.25	0.650
C(11)-N(1)-C(14)-O(3)	-0.8(3)	-0.70	0.100
N(2)-N(1)-C(11)-C(12)	-0.6(2)	0.00	0.600
N(2)-N(1)-C(11)-C(10)	-179.2(2)	-179.86	-0.660
C(14)-N(1)-C(11)-C(12)	-178.7(2)	-179.98	-1.280
C(14)-N(1)-C(11)-C(10)	2.7(3)	0.11	-2.590
N(1)-N(2)-C(13)-C(12)	0.6(2)	0.04	-0.560
C(11)-C(12)-C(7)-C(8)	0.5(3)	0.00	-0.500
C(13)-C(12)-C(7)-C(8)	-179.8(2)	-179.83	-0.030
C(7)-C(12)-C(11)-N(1)	-179.3(2)	-179.86	-0.560
C(7)-C(12)-C(11)-C(10)	-0.5(3)	-0.03	0.470
C(13)-C(12)-C(11)-N(1)	0.9(2)	0.02	-0.880
C(13)-C(12)-C(11)-C(10)	179.7(2)	179.90	0.200
C(7)-C(12)-C(13)-N(2)	179.3(2)	179.81	0.510
C(11)-C(12)-C(13)-N(2)	-1.0(2)	-0.04	0.960
C(12)-C(7)-C(8)-C(9)	-0.0(3)	-0.04	-0.040
C(12)-C(7)-C(8)-B(1)	-178.1(2)	179.91	358.010
N(1)-C(8)-C(9)-C(10)	178.4(2)	179.83	1.430
C(12)-C(11)-C(10)-C(9)	-0.0(3)	-0.02	-0.020
C(7)-C(8)-C(9)-C(10)	-0.5(3)	-0.04	0.460

B(1)-C(8)-C(9)-C(10)	177.6(2)	179.90	2.300
C(7)-C(8)-B(1)-O(2)	12.2(3)	3.07	-9.130
C(7)-C(8)-B(1)-O(1)	-168.4(2)	-176.88	-8.480
C(9)-C(8)-B(1)-O(2)	-165.9(2)	-176.98	-11.080
C(9)-C(8)-B(1)-O(1)	13.6(3)	3.07	-10.530
C(8)-C(9)-C(10)-C(11)	0.5(3)	-0.01	-0.510
O(1)-C(1)-C(5)-O(2)	26.4(2)	26.15	-0.250
O(1)-C(1)-C(5)-C(4)	-88.0(2)	-88.2	-0.200
O(1)-C(1)-C(5)-C(6)	144.1(2)	143.5	-0.600
C(2)-C(11)-C(5)-O(2)	143.9(2)	143.49	-0.410
C(2)-C(11)-C(5)-C(4)	29.4(2)	29.13	-0.270
C(2)-C(11)-C(5)-C(6)	-98.5(2)	-99.16	-0.660
C(3)-C(11)-C(5)-O(2)	-87.7(2)	-88.26	-0.560
Torsion angle (°)	**Exp.[a]**	**Calcd.[b]**	**Difference**
C(3)-C(11)-C(5)-C(4)	157.8(2)	157.38	-0.420
C(3)-C(11)-C(5)-C(6)	29.9(3)	29.09	-0.810

a: Experimental geometry parameters for compound **1**; b: Calculated geometry parameters for conformer **1**.