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Supporting information for article:

Crystal and geometry-optimized structure of an anthracene-based Diels–Alder adduct

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1. NMR, IR, and MS of 1, 17-Ethyl-1-(hydroxymethyl)-17-azapentacyclo[6.6.5.$0^{2,7}$.$0^{9,14}$.$0^{15,19}$]nonadeca-2,4,6,9,11,13-hexaene-16,18-dione

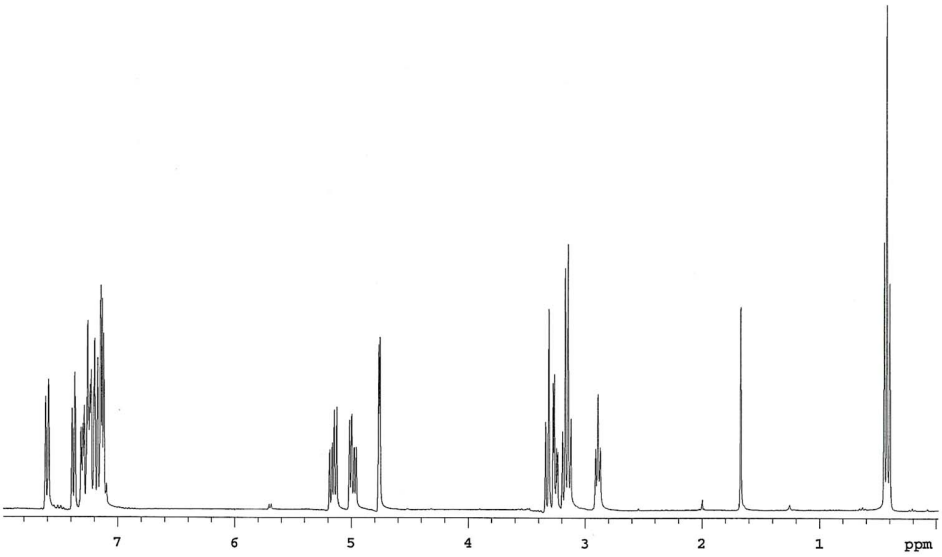

Figure S1: ^{1}H-NMR spectrum of **1** in $CDCl_3$ at 300 MHz

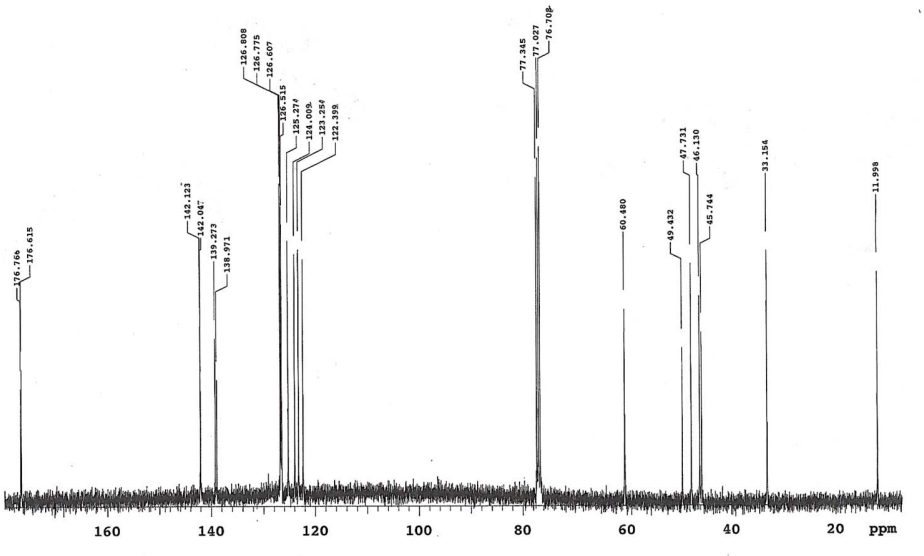

Figure S2: ^{13}C-NMR spectrum of **1** in $CDCl_3$ at 125 MHz

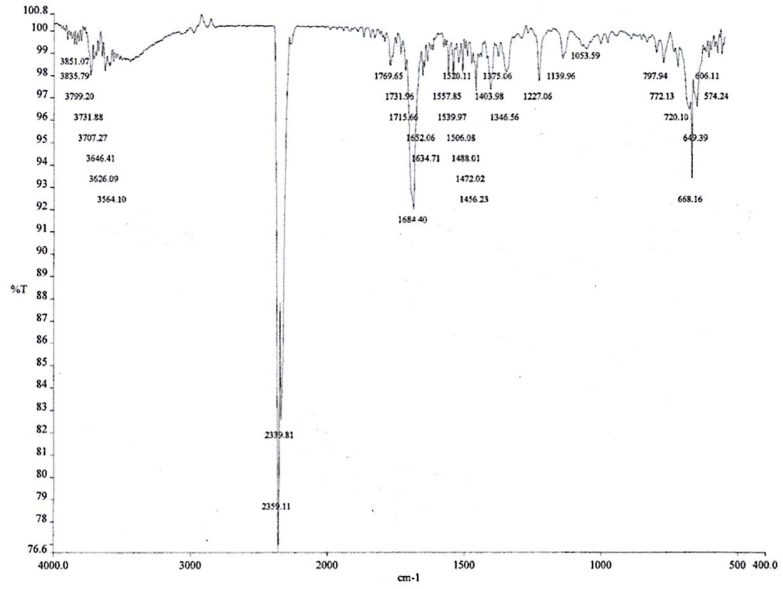

Figure S3: IR spectrum of **1**

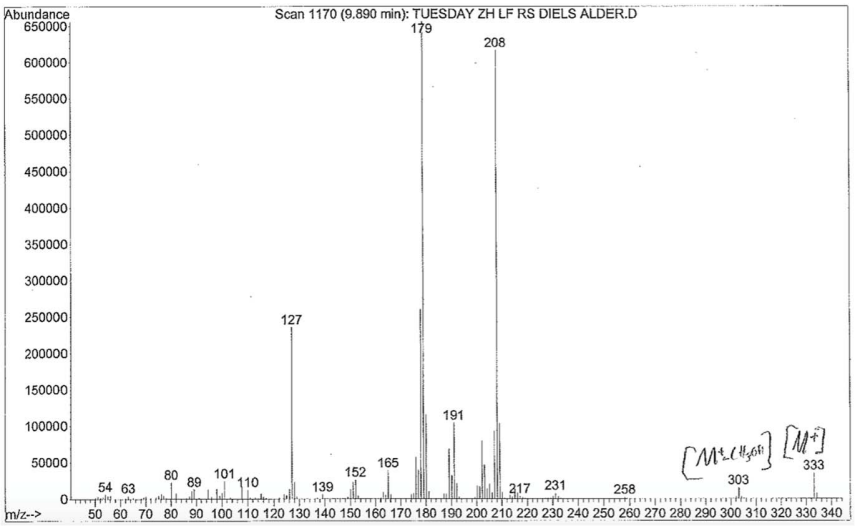

Figure S4: Mass spectrum of **1** with molecular ion peak at *m/z* 333

2. Crystal data and structure refinement for 1

Table S1: Crystal data and structure refinement for **1**

Identification code	AR2009C
Chemical formula	$C_{21}H_{19}NO_3$

Formula weight	333.37 g/mol	
Temperature	125(2) K	
Wavelength	0.71073 Å	
Crystal size	0.200 x 0.260 x 0.330 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 12.2110(13) Å	α = 90°
	b = 8.1447(9) Å	β = 109.430(2)°
	c = 17.6634(19) Å	γ = 90°
Volume	1656.7(3) $Å^3$	
Z	4	
Density (calculated)	1.337 g/cm^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	704	

Theta range for data collection	1.77 to 31.52°
Index ranges	-17<=h<=17, -11<=k<=11, -25<=l<=25
Reflections collected	36543
Independent reflections	5486 [R(int) = 0.0281]
Coverage of independent reflections	99.4%
Absorption correction	multi-scan
Max. and min. transmission	0.9800 and 0.9000
Structure solution technique	direct methods
Structure solution program	SHELXT2014 (Sheldrick, 2015)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL2014/6 (Sheldrick, 2015)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	5486 / 1 / 230
Goodness-of-fit on F^2	1.022

Δ/σ_{max}	0.001	
Final R indices	4784 data; I>2σ(I)	R1 = 0.0386, wR2 = 0.1043
	all data	R1 = 0.0450, wR2 = 0.1098
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0633P)^2+0.4753P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.499 and -0.219 eÅ^{-3}	
R.M.S. deviation from mean	0.053 eÅ^{-3}	

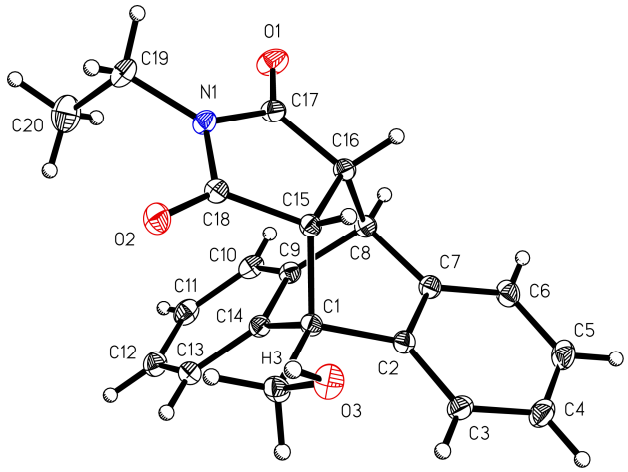

Figure S5: Crystal structure of **1**

Table S2. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
O1	0.73973(6)	0.96692(8)	0.50764(4)	0.02254(15)
O2	0.85332(6)	0.43164(8)	0.53871(4)	0.01947(14)
O3	0.64094(6)	0.20767(8)	0.58591(4)	0.01919(14)
N1	0.81304(6)	0.70584(9)	0.51418(4)	0.01427(14)
C1	0.68346(7)	0.48699(9)	0.63505(5)	0.01212(14)
C2	0.56498(7)	0.52050(10)	0.64336(5)	0.01331(14)
C3	0.49221(7)	0.40476(11)	0.66004(5)	0.01628(16)

	x/a	y/b	z/c	U(eq)
C4	0.38528(8)	0.45515(12)	0.66472(5)	0.01995(17)
C5	0.35126(8)	0.61850(13)	0.65242(6)	0.02073(18)
C6	0.42446(7)	0.73570(11)	0.63676(5)	0.01791(16)
C7	0.53159(7)	0.68625(10)	0.63305(5)	0.01386(15)
C8	0.62088(7)	0.79749(10)	0.61719(5)	0.01353(14)
C9	0.73581(7)	0.76794(10)	0.68294(5)	0.01299(14)
C10	0.80741(8)	0.88879(10)	0.72961(5)	0.01651(16)
C11	0.91105(8)	0.84398(12)	0.78889(5)	0.01926(17)
C12	0.94309(8)	0.67986(12)	0.80034(5)	0.01901(17)
C13	0.87269(7)	0.55800(11)	0.75254(5)	0.01583(15)
C14	0.76898(7)	0.60215(10)	0.69361(5)	0.01276(14)
C15	0.67343(7)	0.55010(9)	0.54881(5)	0.01195(14)
C16	0.63540(7)	0.73176(10)	0.53816(5)	0.01289(14)
C17	0.73168(7)	0.81973(10)	0.51840(5)	0.01469(15)
C18	0.78911(7)	0.54773(10)	0.53426(5)	0.01320(14)
C19	0.91711(8)	0.74664(11)	0.49436(6)	0.01882(17)
C20	0.01784(9)	0.79573(14)	0.56769(7)	0.0291(2)
C21	0.71934(7)	0.30681(10)	0.64652(5)	0.01569(15)

Table S3. Bond lengths (Å) for **1**.

O1-C17	1.2229(10)	O2-C18	1.2140(10)
O3-C21	1.4257(10)	O3-H3	0.830(12)
N1-C17	1.3792(10)	N1-C18	1.3923(11)
N1-C19	1.4643(11)	C1-C14	1.5237(11)
C1-C21	1.5256(11)	C1-C2	1.5266(11)
C1-C15	1.5734(11)	C2-C3	1.3926(11)
C2-C7	1.4044(11)	C3-C4	1.3971(12)
C3-H3B	0.95	C4-C5	1.3891(14)
C4-H4A	0.95	C5-C6	1.3969(13)
C5-H5A	0.95	C6-C7	1.3910(11)
C6-H6A	0.95	C7-C8	1.5137(11)
C8-C9	1.5139(11)	C8-C16	1.5592(11)
C8-H8A	1.0	C9-C10	1.3904(11)
C9-C14	1.4044(11)	C10-C11	1.3963(13)

C10-H10A	0.95	C11-C12	1.3886(13)
C11-H11A	0.95	C12-C13	1.3979(12)
C12-H12A	0.95	C13-C14	1.3926(11)
C13-H13A	0.95	C15-C18	1.5177(11)
C15-C16	1.5434(11)	C15-H15A	1.0
C16-C17	1.5134(11)	C16-H16A	1.0
C19-C20	1.5135(14)	C19-H19A	0.99
C19-H19B	0.99	C20-H20A	0.98
C20-H20B	0.98	C20-H20C	0.98
C21-H21A	0.99	C21-H21B	0.99

Table S4. Bond angles (°) for **1**.

C21-O3-H3	111.2(9)	C17-N1-C18	113.10(7)
C17-N1-C19	123.94(7)	C18-N1-C19	122.90(7)
C14-C1-C21	113.59(7)	C14-C1-C2	106.38(6)
C21-C1-C2	113.50(7)	C14-C1-C15	105.74(6)
C21-C1-C15	111.67(6)	C2-C1-C15	105.29(6)
C3-C2-C7	120.00(7)	C3-C2-C1	126.24(7)
C7-C2-C1	113.76(7)	C2-C3-C4	119.23(8)
C2-C3-H3B	120.4	C4-C3-H3B	120.4
C5-C4-C3	120.58(8)	C5-C4-H4A	119.7
C3-C4-H4A	119.7	C4-C5-C6	120.51(8)
C4-C5-H5A	119.7	C6-C5-H5A	119.7
C7-C6-C5	119.03(8)	C7-C6-H6A	120.5
C5-C6-H6A	120.5	C6-C7-C2	120.61(8)
C6-C7-C8	125.59(8)	C2-C7-C8	113.79(7)
C7-C8-C9	107.68(7)	C7-C8-C16	105.28(6)
C9-C8-C16	106.25(6)	C7-C8-H8A	112.4
C9-C8-H8A	112.4	C16-C8-H8A	112.4
C10-C9-C14	120.31(8)	C10-C9-C8	125.58(7)
C14-C9-C8	114.09(7)	C9-C10-C11	119.60(8)
C9-C10-H10A	120.2	C11-C10-H10A	120.2
C12-C11-C10	120.13(8)	C12-C11-H11A	119.9
C10-C11-H11A	119.9	C11-C12-C13	120.58(8)
C11-C12-H12A	119.7	C13-C12-H12A	119.7
C14-C13-C12	119.45(8)	C14-C13-H13A	120.3
C12-C13-H13A	120.3	C13-C14-C9	119.91(7)
C13-C14-C1	126.58(7)	C9-C14-C1	113.50(7)
C18-C15-C16	104.53(6)	C18-C15-C1	112.50(6)
C16-C15-C1	110.76(6)	C18-C15-H15A	109.6
C16-C15-H15A	109.6	C1-C15-H15A	109.6
C17-C16-C15	104.87(6)	C17-C16-C8	111.86(7)
C15-C16-C8	109.83(6)	C17-C16-H16A	110.1
C15-C16-H16A	110.1	C8-C16-H16A	110.1

O1-C17-N1	123.67(8)	O1-C17-C16	127.49(8)
N1-C17-C16	108.84(7)	O2-C18-N1	123.44(8)
O2-C18-C15	128.05(8)	N1-C18-C15	108.50(6)
N1-C19-C20	112.22(8)	N1-C19-H19A	109.2
C20-C19-H19A	109.2	N1-C19-H19B	109.2
C20-C19-H19B	109.2	H19A-C19-H19B	107.9
C19-C20-H20A	109.5	C19-C20-H20B	109.5
H20A-C20-H20B	109.5	C19-C20-H20C	109.5
H20A-C20-H20C	109.5	H20B-C20-H20C	109.5
O3-C21-C1	110.71(7)	O3-C21-H21A	109.5
C1-C21-H21A	109.5	O3-C21-H21B	109.5
C1-C21-H21B	109.5	H21A-C21-H21B	108.1

Table S5. Torsion angles (°) for **1**.

C14-C1-C2-C3	-125.36(8)	C21-C1-C2-C3	0.28(12)
C15-C1-C2-C3	122.71(8)	C14-C1-C2-C7	54.22(9)
C21-C1-C2-C7	179.86(7)	C15-C1-C2-C7	-57.71(8)
C7-C2-C3-C4	1.27(12)	C1-C2-C3-C4	-179.18(8)
C2-C3-C4-C5	0.40(13)	C3-C4-C5-C6	-1.29(14)
C4-C5-C6-C7	0.48(13)	C5-C6-C7-C2	1.20(13)
C5-C6-C7-C8	-179.64(8)	C3-C2-C7-C6	-2.09(12)
C1-C2-C7-C6	178.31(7)	C3-C2-C7-C8	178.66(7)
C1-C2-C7-C8	-0.94(10)	C6-C7-C8-C9	128.23(8)
C2-C7-C8-C9	-52.57(9)	C6-C7-C8-C16	-118.72(9)
C2-C7-C8-C16	60.49(8)	C7-C8-C9-C10	-128.93(8)
C16-C8-C9-C10	118.67(8)	C7-C8-C9-C14	52.38(9)
C16-C8-C9-C14	-60.03(8)	C14-C9-C10-C11	-1.91(12)
C8-C9-C10-C11	179.47(8)	C9-C10-C11-C12	0.91(13)
C10-C11-C12-C13	0.41(13)	C11-C12-C13-C14	-0.71(13)
C12-C13-C14-C9	-0.29(12)	C12-C13-C14-C1	178.42(8)
C10-C9-C14-C13	1.61(12)	C8-C9-C14-C13	-179.62(7)
C10-C9-C14-C1	-177.27(7)	C8-C9-C14-C1	1.51(10)
C21-C1-C14-C13	1.20(11)	C2-C1-C14-C13	126.79(8)
C15-C1-C14-C13	-121.59(8)	C21-C1-C14-C9	179.99(7)
C2-C1-C14-C9	-54.43(9)	C15-C1-C14-C9	57.19(8)
C14-C1-C15-C18	59.80(8)	C21-C1-C15-C18	-64.22(8)
C2-C1-C15-C18	172.18(6)	C14-C1-C15-C16	-56.78(8)
C21-C1-C15-C16	179.21(6)	C2-C1-C15-C16	55.60(8)
C18-C15-C16-C17	-0.01(8)	C1-C15-C16-C17	121.39(7)
C18-C15-C16-C8	-120.36(7)	C1-C15-C16-C8	1.04(9)
C7-C8-C16-C17	-174.10(6)	C9-C8-C16-C17	-60.04(8)
C7-C8-C16-C15	-58.08(8)	C9-C8-C16-C15	55.97(8)
C18-N1-C17-O1	175.69(8)	C19-N1-C17-O1	-1.61(13)
C18-N1-C17-C16	-4.18(9)	C19-N1-C17-C16	178.52(7)

C15-C16-C17-O1	-177.46(9)	C8-C16-C17-O1	-58.47(11)
C15-C16-C17-N1	2.39(8)	C8-C16-C17-N1	121.39(7)
C17-N1-C18-O2	-175.69(8)	C19-N1-C18-O2	1.65(13)
C17-N1-C18-C15	4.16(9)	C19-N1-C18-C15	-178.50(7)
C16-C15-C18-O2	177.49(8)	C1-C15-C18-O2	57.24(11)
C16-C15-C18-N1	-2.35(8)	C1-C15-C18-N1	-122.60(7)
C17-N1-C19-C20	87.01(10)	C18-N1-C19-C20	-90.04(10)
C14-C1-C21-O3	-175.24(7)	C2-C1-C21-O3	63.06(9)
C15-C1-C21-O3	-55.77(9)		

Table S6. Hydrogen bond distances (Å) and angles (°) for **1**.

	Donor-H	**Acceptor-H**	**Donor-Acceptor**	**Angle**
O3-H3···O1	0.830(12)	2.078(12)	2.8846(10)	164.0(13)

Table S7. Anisotropic atomic displacement parameters (Å^2) for **1**.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	0.0308(4)	0.0125(3)	0.0299(4)	0.0041(2)	0.0174(3)	0.0021(2)
O2	0.0193(3)	0.0163(3)	0.0251(3)	0.0001(2)	0.0104(2)	0.0056(2)
O3	0.0195(3)	0.0121(3)	0.0267(3)	-0.0046(2)	0.0085(2)	-0.0006(2)
N1	0.0149(3)	0.0134(3)	0.0166(3)	-0.0003(2)	0.0081(2)	0.0003(2)
C1	0.0122(3)	0.0099(3)	0.0142(3)	0.0006(2)	0.0044(3)	0.0011(2)
C2	0.0126(3)	0.0144(3)	0.0132(3)	0.0006(3)	0.0047(3)	0.0009(3)
C3	0.0170(4)	0.0173(4)	0.0157(3)	0.0012(3)	0.0069(3)	-0.0015(3)
C4	0.0175(4)	0.0266(4)	0.0183(4)	-0.0004(3)	0.0093(3)	-0.0036(3)
C5	0.0151(4)	0.0297(5)	0.0197(4)	-0.0020(3)	0.0090(3)	0.0017(3)
C6	0.0159(4)	0.0211(4)	0.0178(4)	-0.0003(3)	0.0070(3)	0.0049(3)
C7	0.0140(3)	0.0145(3)	0.0139(3)	-0.0001(3)	0.0056(3)	0.0018(3)
C8	0.0146(3)	0.0110(3)	0.0161(3)	0.0003(3)	0.0066(3)	0.0025(3)
C9	0.0142(3)	0.0121(3)	0.0138(3)	-0.0004(3)	0.0063(3)	0.0004(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C10	0.0202(4)	0.0140(3)	0.0177(4)	-0.0025(3)	0.0094(3)	-0.0029(3)
C11	0.0189(4)	0.0216(4)	0.0179(4)	-0.0041(3)	0.0071(3)	-0.0064(3)
C12	0.0150(4)	0.0246(4)	0.0162(4)	0.0005(3)	0.0036(3)	-0.0029(3)
C13	0.0144(3)	0.0176(4)	0.0152(3)	0.0021(3)	0.0046(3)	0.0008(3)
C14	0.0128(3)	0.0127(3)	0.0134(3)	0.0002(3)	0.0053(3)	0.0001(3)
C15	0.0120(3)	0.0105(3)	0.0137(3)	0.0002(2)	0.0046(3)	0.0016(2)
C16	0.0136(3)	0.0114(3)	0.0144(3)	0.0014(3)	0.0057(3)	0.0025(3)
C17	0.0176(4)	0.0132(3)	0.0145(3)	0.0009(3)	0.0070(3)	0.0018(3)
C18	0.0141(3)	0.0128(3)	0.0130(3)	-0.0011(3)	0.0049(3)	0.0005(3)
C19	0.0187(4)	0.0198(4)	0.0222(4)	-0.0009(3)	0.0125(3)	-0.0020(3)
C20	0.0205(4)	0.0314(5)	0.0344(5)	-0.0059(4)	0.0078(4)	-0.0062(4)
C21	0.0162(4)	0.0106(3)	0.0194(4)	0.0012(3)	0.0049(3)	0.0015(3)

Table S8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for **1**.

	x/a	y/b	z/c	U(eq)
H3	0.6757(11)	0.1545(16)	0.5608(8)	0.023
H3B	0.5150	0.2928	0.6681	0.02
H4A	0.3354	0.3770	0.6764	0.024
H5A	0.2777	0.6508	0.6547	0.025
H6A	0.4014	0.8475	0.6288	0.021
H8A	0.5972	0.9156	0.6130	0.016
H10A	0.7859	1.0012	0.7212	0.02
H11A	0.9597	0.9259	0.8215	0.023
H12A	1.0135	0.6501	0.8410	0.023
H13A	0.8954	0.4460	0.7602	0.019
H15A	0.6158	0.4816	0.5073	0.014
H16A	0.5606	0.7430	0.4927	0.015
H19A	0.8990	0.8381	0.4552	0.023
H19B	0.9399	0.6504	0.4687	0.023
H20A	1.0848	0.8246	0.5515	0.044

	x/a	y/b	z/c	U(eq)
H20B	1.0384	0.7038	0.6056	0.044
H20C	0.9955	0.8906	0.5934	0.044
H21A	0.7988	0.2945	0.6442	0.019
H21B	0.7202	0.2694	0.7000	0.019

3. Computational Calculations at the B2PLYPD3/6-311++G(2d,2p)//B3LYP/6-31+G(d,p) Level of Theory

1a.

SCF E(RB3LYP) = -1092.21461986 a.u.

Zero-point correction= 0.358477 (Hartree/Particle)
Thermal correction to Energy= 0.378376
Thermal correction to Enthalpy= 0.379320
Thermal correction to Gibbs Free Energy= 0.310435
Sum of electronic and zero-point Energies= -1091.856142
Sum of electronic and thermal Energies= -1091.836244
Sum of electronic and thermal Enthalpies= -1091.835300
Sum of electronic and thermal Free Energies= -1091.904185

E(B2PLYPD3) = -1091.538475 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.519046	0.382535	-0.229121
2	6	0	3.362320	0.875978	0.389791
3	6	0	2.124091	0.312830	0.084436
4	6	0	2.043390	-0.726270	-0.862698
5	6	0	3.192766	-1.211287	-1.481791
6	6	0	4.437678	-0.657048	-1.157257
7	6	0	0.762114	0.730898	0.660901
8	6	0	0.626318	-1.210986	-1.118471
9	6	0	0.026522	-1.583548	0.221733
10	6	0	0.096715	-0.552893	1.178378
11	6	0	-0.406518	-0.776945	2.462346
12	1	0	-0.358443	-0.007267	3.225245
13	6	0	-0.975478	-2.016529	2.782962

14	6	0	-1.052856	-3.028977	1.825170
15	6	0	-0.552446	-2.810978	0.536330
16	1	0	5.483726	0.818499	0.013804
17	1	0	3.437231	1.702354	1.088622
18	1	0	3.122892	-2.016706	-2.208754
19	1	0	5.338566	-1.034840	-1.631943
20	1	0	0.579448	-2.029292	-1.840108
21	1	0	-1.357099	-2.186635	3.785510
22	1	0	-1.497574	-3.986690	2.079172
23	1	0	-0.611300	-3.592246	-0.216711
24	6	0	-1.653466	-0.191315	-1.801819
25	6	0	-0.153909	0.039757	-1.643653
26	6	0	-0.039179	1.194727	-0.625278
27	6	0	-1.473439	1.611948	-0.347388
28	7	0	-2.329939	0.764426	-1.035745
29	1	0	0.243807	0.317947	-2.625038
30	1	0	0.489600	2.059701	-1.033024
31	8	0	-1.833798	2.552714	0.346988
32	8	0	-2.201648	-1.032684	-2.487367
33	6	0	-3.791110	0.868081	-0.985173
34	1	0	-4.161053	0.558053	-1.965584
35	1	0	-4.024600	1.924509	-0.831798
36	6	0	-4.403078	0.007171	0.121992
37	1	0	-5.492310	0.118354	0.113134
38	1	0	-4.035880	0.314401	1.105327
39	1	0	-4.165053	-1.049456	-0.028487
40	6	0	0.815644	1.847311	1.720776
41	1	0	1.599392	1.619361	2.450151
42	1	0	-0.136618	1.883334	2.256908
43	8	0	1.106103	3.131370	1.179051
44	1	0	0.259755	3.519515	0.909135

1b.

SCF E(RB3LYP) = -1092.21053086 a.u.

Zero-point correction= 0.358047 (Hartree/Particle)
Thermal correction to Energy= 0.378055
Thermal correction to Enthalpy= 0.378999
Thermal correction to Gibbs Free Energy= 0.310221
Sum of electronic and zero-point Energies= -1091.852484
Sum of electronic and thermal Energies= -1091.832476
Sum of electronic and thermal Enthalpies= -1091.831531
Sum of electronic and thermal Free Energies= -1091.900310

E(B2PLYPD3) = -1091.535152 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.325722	-1.178360	-0.675084
2	6	0	3.274367	-0.395421	-1.173051
3	6	0	2.063184	-0.330307	-0.479988
4	6	0	1.900994	-1.090599	0.693518
5	6	0	2.941617	-1.875084	1.184038
6	6	0	4.164885	-1.908650	0.502597
7	6	0	0.810900	0.468689	-0.886713
8	6	0	0.507256	-0.999921	1.281663
9	6	0	0.185230	0.465041	1.496712
10	6	0	0.351823	1.258777	0.346742
11	6	0	0.063954	2.624348	0.401884
12	1	0	0.203438	3.249185	-0.472330
13	6	0	-0.377687	3.188908	1.605091
14	6	0	-0.538484	2.398122	2.745318
15	6	0	-0.260926	1.027678	2.691529
16	1	0	5.267491	-1.216077	-1.214588
17	1	0	3.416617	0.137315	-2.109387
18	1	0	2.802439	-2.459044	2.090347
19	1	0	4.983057	-2.510991	0.886144
20	1	0	0.387268	-1.594219	2.189970
21	1	0	-0.592033	4.252842	1.648797
22	1	0	-0.879517	2.845109	3.674670
23	1	0	-0.394767	0.402961	3.570741
24	6	0	-1.914816	-1.435295	0.528548
25	6	0	-0.441608	-1.528162	0.150983
26	6	0	-0.291631	-0.649629	-1.116402
27	6	0	-1.699991	-0.108218	-1.371196
28	7	0	-2.553973	-0.608042	-0.390999
29	1	0	-0.207282	-2.579593	-0.040991
30	1	0	-0.001615	-1.238673	-1.993062
31	8	0	-2.058114	0.613206	-2.285033
32	8	0	-2.465265	-1.988288	1.462760
33	6	0	-3.984697	-0.295454	-0.335675
34	1	0	-4.480703	-1.174523	0.083007
35	1	0	-4.314627	-0.154463	-1.367770
36	6	0	-4.279905	0.948131	0.505520
37	1	0	-5.358095	1.138884	0.512921
38	1	0	-3.778478	1.827495	0.091790
39	1	0	-3.948873	0.807893	1.538262
40	6	0	1.006419	1.309678	-2.157785
41	1	0	0.058254	1.756221	-2.458572

42	1	0	1.324047	0.647103	-2.976912
43	8	0	1.918435	2.396402	-2.005979
44	1	0	2.735569	2.083896	-1.596306

1c.

SCF E(RB3LYP) = -1092.21526513 a.u.

Zero-point correction= 0.358913 (Hartree/Particle)
Thermal correction to Energy= 0.378460
Thermal correction to Enthalpy= 0.379404
Thermal correction to Gibbs Free Energy= 0.311802
Sum of electronic and zero-point Energies= -1091.856353
Sum of electronic and thermal Energies= -1091.836805
Sum of electronic and thermal Enthalpies= -1091.835861
Sum of electronic and thermal Free Energies= -1091.903463

E(B2PLYPD3) = -1091.538449 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.596748	0.284731	-0.298619
2	6	0	3.412489	1.034647	-0.281561
3	6	0	2.181484	0.389697	-0.141933
4	6	0	2.150648	-1.012955	-0.029092
5	6	0	3.325971	-1.758934	-0.052295
6	6	0	4.557202	-1.105097	-0.183891
7	6	0	0.789938	1.058375	-0.095764
8	6	0	0.749712	-1.577152	0.090633
9	6	0	0.072772	-0.876117	1.252480
10	6	0	0.099271	0.529678	1.168893
11	6	0	-0.468151	1.292736	2.192626
12	1	0	-0.476471	2.374059	2.123653
13	6	0	-1.048742	0.648636	3.292843
14	6	0	-1.079149	-0.745595	3.368396
15	6	0	-0.519176	-1.513744	2.341232
16	1	0	5.550329	0.794647	-0.399889
17	1	0	3.474751	2.113426	-0.372659
18	1	0	3.285221	-2.841678	0.036382
19	1	0	5.478609	-1.679848	-0.195049
20	1	0	0.734539	-2.664622	0.190491
21	1	0	-1.483411	1.243862	4.090820
22	1	0	-1.535270	-1.235517	4.223822

23	1	0	-0.538306	-2.599310	2.391063
24	6	0	-1.434306	-1.551602	-1.267300
25	6	0	0.028607	-1.136343	-1.224031
26	6	0	0.021700	0.409692	-1.329609
27	6	0	-1.461666	0.760370	-1.460073
28	7	0	-2.211820	-0.400205	-1.416770
29	1	0	0.533093	-1.604838	-2.074884
30	1	0	0.513013	0.758018	-2.244795
31	8	0	-1.948956	1.872483	-1.623911
32	8	0	-1.882355	-2.679557	-1.203784
33	6	0	-3.675532	-0.421210	-1.511169
34	1	0	-3.941795	-1.376180	-1.970137
35	1	0	-3.959655	0.392091	-2.183084
36	6	0	-4.350403	-0.263653	-0.146958
37	1	0	-5.437807	-0.287913	-0.271832
38	1	0	-4.079640	0.689388	0.315719
39	1	0	-4.064157	-1.076115	0.526721
40	6	0	0.919856	2.594406	-0.194299
41	1	0	1.396361	2.836183	-1.157521
42	1	0	1.598733	2.928903	0.596430
43	8	0	-0.264080	3.345289	-0.019387
44	1	0	-0.919049	3.071032	-0.687856

1d.

SCF E(RB3LYP) = -1092.21462891 a.u.

Zero-point correction= 0.358441 (Hartree/Particle)
Thermal correction to Energy= 0.378356
Thermal correction to Enthalpy= 0.379301
Thermal correction to Gibbs Free Energy= 0.310398
Sum of electronic and zero-point Energies= -1091.856188
Sum of electronic and thermal Energies= -1091.836272
Sum of electronic and thermal Enthalpies= -1091.835328
Sum of electronic and thermal Free Energies= -1091.904231

E(B2PLYPD3) = -1091.537743 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.525834	-0.364088	-0.232677
2	6	0	-3.375640	-0.858650	0.397484
3	6	0	-2.131872	-0.309361	0.089525

4	6	0	-2.038865	0.714693	-0.872800
5	6	0	-3.181702	1.200336	-1.503371
6	6	0	-4.432454	0.661386	-1.175241
7	6	0	-0.775960	-0.731624	0.675292
8	6	0	-0.616437	1.182781	-1.131414
9	6	0	-0.016324	1.569234	0.204486
10	6	0	-0.097568	0.552875	1.175129
11	6	0	0.410622	0.788279	2.455125
12	1	0	0.356998	0.029093	3.227999
13	6	0	0.992872	2.025991	2.758526
14	6	0	1.079206	3.024877	1.787374
15	6	0	0.575510	2.794686	0.501984
16	1	0	-5.495098	-0.788355	0.012762
17	1	0	-3.458888	-1.675611	1.106489
18	1	0	-3.102112	1.993869	-2.242317
19	1	0	-5.328443	1.039797	-1.658624
20	1	0	-0.559585	1.989694	-1.865073
21	1	0	1.378615	2.204944	3.757932
22	1	0	1.535471	3.980695	2.027600
23	1	0	0.643330	3.564435	-0.262045
24	6	0	1.659621	0.136646	-1.777876
25	6	0	0.156594	-0.082222	-1.634425
26	6	0	0.022520	-1.223171	-0.603172
27	6	0	1.449738	-1.653976	-0.311998
28	7	0	2.320114	-0.817545	-0.995811
29	1	0	-0.233655	-0.369401	-2.616287
30	1	0	-0.516660	-2.086058	-1.001264
31	8	0	1.795504	-2.589260	0.397079
32	8	0	2.221774	0.973808	-2.457100
33	6	0	3.779602	-0.921570	-0.915014
34	1	0	4.012820	-1.295923	0.084550
35	1	0	4.170593	0.093629	-1.017018
36	6	0	4.363269	-1.840247	-1.990677
37	1	0	5.452538	-1.880970	-1.888233
38	1	0	4.129818	-1.467005	-2.992118
39	1	0	3.973747	-2.857563	-1.889868
40	6	0	-0.842937	-1.828740	1.753966
41	1	0	-1.619354	-1.574444	2.482539
42	1	0	0.111209	-1.871343	2.286040
43	8	0	-1.158895	-3.117018	1.236784
44	1	0	-0.320978	-3.525417	0.970846

1e.

SCF E(RB3LYP) = -1092.21051719 a.u.

Zero-point correction= 0.357923 (Hartree/Particle)
Thermal correction to Energy= 0.377960
Thermal correction to Enthalpy= 0.378904
Thermal correction to Gibbs Free Energy= 0.310029
Sum of electronic and zero-point Energies= -1091.852594
Sum of electronic and thermal Energies= -1091.832558
Sum of electronic and thermal Enthalpies= -1091.831613
Sum of electronic and thermal Free Energies= -1091.900488

E(B2PLYPD3) = -1091.534218 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.326386	-1.169813	-0.693748
2	6	0	3.270233	-0.386034	-1.179870
3	6	0	2.063528	-0.327825	-0.478442
4	6	0	1.910562	-1.095201	0.691593
5	6	0	2.955810	-1.880882	1.170202
6	6	0	4.174505	-1.908113	0.480215
7	6	0	0.805512	0.467285	-0.874950
8	6	0	0.519868	-1.013492	1.287236
9	6	0	0.188451	0.447961	1.510388
10	6	0	0.345735	1.248118	0.363708
11	6	0	0.043987	2.610448	0.425049
12	1	0	0.175014	3.240158	-0.446867
13	6	0	-0.404233	3.164764	1.630519
14	6	0	-0.556825	2.367356	2.767211
15	6	0	-0.263907	1.000363	2.707624
16	1	0	5.264581	-1.202731	-1.239760
17	1	0	3.404562	0.152520	-2.113917
18	1	0	2.823342	-2.471391	2.073287
19	1	0	4.996006	-2.511927	0.854204
20	1	0	0.407208	-1.613169	2.192979
21	1	0	-0.631262	4.225869	1.678401
22	1	0	-0.904125	2.806318	3.698033
23	1	0	-0.391899	0.370102	3.583681
24	6	0	-1.902784	-1.453208	0.546447
25	6	0	-0.432154	-1.540840	0.158181
26	6	0	-0.292690	-0.656038	-1.106189
27	6	0	-1.705007	-0.119712	-1.350839
28	7	0	-2.550718	-0.625631	-0.366763
29	1	0	-0.195178	-2.590633	-0.039692
30	1	0	-0.003376	-1.238684	-1.987457
31	8	0	-2.070995	0.609164	-2.255612

32	8	0	-2.443526	-2.003317	1.487933
33	6	0	-3.979436	-0.308540	-0.294541
34	1	0	-4.095419	0.708116	-0.677323
35	1	0	-4.249703	-0.326191	0.763866
36	6	0	-4.838794	-1.292099	-1.091928
37	1	0	-5.893801	-1.011874	-1.007161
38	1	0	-4.725550	-2.310322	-0.708011
39	1	0	-4.567365	-1.278483	-2.151596
40	6	0	0.990066	1.315934	-2.142682
41	1	0	0.037734	1.759169	-2.434926
42	1	0	1.305872	0.658942	-2.967069
43	8	0	1.897756	2.406148	-1.990469
44	1	0	2.719623	2.095086	-1.589248

1f.

SCF E(RB3LYP) = -1092.21530519 a.u.

Zero-point correction= 0.358738 (Hartree/Particle)
Thermal correction to Energy= 0.378328
Thermal correction to Enthalpy= 0.379273
Thermal correction to Gibbs Free Energy= 0.311384
Sum of electronic and zero-point Energies= -1091.856567
Sum of electronic and thermal Energies= -1091.836977
Sum of electronic and thermal Enthalpies= -1091.836033
Sum of electronic and thermal Free Energies= -1091.903921

E(B2PLYPD3) = -1091.537691 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.395938	-0.878122	-1.025539
2	6	0	3.282981	-0.101203	-1.375986
3	6	0	2.105616	-0.193946	-0.630150
4	6	0	2.053936	-1.079564	0.462322
5	6	0	3.157160	-1.855373	0.808024
6	6	0	4.337149	-1.750652	0.061454
7	6	0	0.797811	0.592462	-0.869030
8	6	0	0.710092	-1.096145	1.160715
9	6	0	0.374434	0.332097	1.544492
10	6	0	0.431359	1.242872	0.471618
11	6	0	0.162855	2.595162	0.698421
12	1	0	0.177900	3.297781	-0.126375

13	6	0	-0.152995	3.028046	1.992719
14	6	0	-0.215600	2.120644	3.052453
15	6	0	0.045885	0.764166	2.828150
16	1	0	5.309782	-0.794399	-1.606462
17	1	0	3.359259	0.567722	-2.226043
18	1	0	3.101656	-2.532986	1.656299
19	1	0	5.204199	-2.346924	0.330022
20	1	0	0.679737	-1.777881	2.013423
21	1	0	-0.356442	4.080553	2.168210
22	1	0	-0.466395	2.465453	4.051457
23	1	0	-0.002118	0.050689	3.646623
24	6	0	-1.742344	-1.567019	0.555838
25	6	0	-0.304616	-1.550078	0.060486
26	6	0	-0.286438	-0.545147	-1.120080
27	6	0	-1.739413	-0.076057	-1.221923
28	7	0	-2.491422	-0.700339	-0.243959
29	1	0	-0.046915	-2.565310	-0.256891
30	1	0	-0.040617	-1.034344	-2.069104
31	8	0	-2.213489	0.697841	-2.044977
32	8	0	-2.195977	-2.213871	1.479469
33	6	0	-3.926744	-0.467260	-0.053527
34	1	0	-4.118561	0.567085	-0.347381
35	1	0	-4.118521	-0.577803	1.016268
36	6	0	-4.789868	-1.435904	-0.864580
37	1	0	-5.848457	-1.225308	-0.681634
38	1	0	-4.594340	-2.472031	-0.572975
39	1	0	-4.601490	-1.325356	-1.936466
40	6	0	0.957959	1.560887	-2.062001
41	1	0	1.181946	0.962643	-2.959458
42	1	0	1.829227	2.194517	-1.868720
43	8	0	-0.110353	2.451473	-2.309191
44	1	0	-0.928884	1.939920	-2.450011
