

Supplementary Data

Synthesis of *N*-(Anthracen-9-ylmethyl)-*N*-methyl-2-(phenylsulfonyl)ethanamine Via Microwave Green Synthesis Method: X-Ray Characterization, DFT and Hirshfeld Analysis

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Table S1 The calculated bond distances and angles compared to the experimental data of aza-Michael product **3^a**.

Parameter	Calc.	Exp.
R(1-2)	1.530	1.550
R(1-35)	1.464	1.473
R(2-3)	1.822	1.778
R(3-4)	1.473	1.470
R(3-5)	1.473	1.470
R(3-6)	1.804	1.773
R(6-7)	1.396	1.350
R(6-11)	1.396	1.354
R(7-8)	1.395	1.353
R(8-9)	1.396	1.360
R(9-10)	1.397	1.352
R(10-11)	1.395	1.350
R(20-21)	1.423	1.356
R(20-25)	1.370	1.359
R(21-22)	1.367	1.352
R(22-23)	1.430	1.354
R(23-24)	1.449	1.362
R(23-26)	1.396	1.356
R(24-25)	1.436	1.356
R(24-29)	1.418	1.360
R(26-27)	1.397	1.352
R(27-28)	1.444	1.354
R(27-30)	1.430	1.354
R(28-29)	1.418	1.358
R(28-33)	1.433	1.357
R(29-34)	1.519	1.547
R(30-31)	1.368	1.355
R(31-32)	1.423	1.355
R(32-33)	1.371	1.355
R(34-35)	1.476	1.474
R(35-36)	1.459	1.470
A(2-1-12)	107.7	110.0
A(2-1-13)	110.1	110.3
A(2-1-35)	111.0	107.5
A(1-2-3)	113.9	111.2
A(1-2-14)	110.4	108.7
A(1-2-48)	113.9	109.3
A(12-1-13)	107.4	109.1
A(12-1-35)	108.6	110.5

A(13-1-35)	111.9	109.4
A(1-35-34)	113.0	112.8
A(1-35-36)	112.4	107.7
A(3-2-14)	103.8	109.7
A(3-2-48)	105.7	107.9
A(2-3-4)	106.5	109.8
A(2-3-5)	107.9	110.5
A(2-3-6)	105.0	107.4
A(14-2-48)	108.5	110.0
A(4-3-5)	121.3	108.9
A(4-3-6)	107.5	109.6
A(5-3-6)	107.5	110.6
A(3-6-7)	119.3	120.8
A(3-6-11)	119.2	119.0
A(7-6-11)	121.6	120.3
A(6-7-8)	118.9	119.6
A(6-7-15)	119.6	120.0
A(6-11-10)	119.0	120.2
A(6-11-19)	119.8	120.0
A(8-7-15)	121.5	120.4
A(7-8-9)	120.1	120.1
A(7-8-16)	119.8	119.8
A(9-8-16)	120.1	120.1
A(8-9-10)	120.4	120.0
A(8-9-17)	119.8	120.2
A(10-9-17)	119.8	119.9
A(9-10-11)	120.1	119.7
A(9-10-18)	120.1	120.3
A(11-10-18)	119.8	120.0
A(10-11-19)	121.2	119.7
A(21-20-25)	121.0	120.1
A(21-20-37)	119.4	119.7
A(20-21-22)	119.6	120.0
A(20-21-38)	119.9	120.1
A(25-20-37)	119.6	120.1
A(20-25-24)	121.8	119.9
A(20-25-40)	118.5	120.0
A(22-21-38)	120.6	119.9
A(21-22-23)	121.3	120.0
A(21-22-39)	120.7	120.1
A(23-22-39)	118.0	119.9
A(22-23-24)	119.7	120.2
A(22-23-26)	120.7	119.5

A(24-23-26)	119.6	120.3
A(23-24-25)	116.7	119.7
A(23-24-29)	119.5	119.5
A(23-26-27)	121.7	120.1
A(23-26-41)	119.1	120.0
A(25-24-29)	123.8	120.7
A(24-25-40)	119.7	120.1
A(24-29-28)	119.9	119.7
A(24-29-34)	121.3	122.4
A(27-26-41)	119.2	120.0
A(26-27-28)	119.3	119.8
A(26-27-30)	121.2	119.9
A(28-27-30)	119.5	120.2
A(27-28-29)	119.9	120.5
A(27-28-33)	117.4	119.8
A(27-30-31)	121.1	120.0
A(27-30-42)	118.2	120.1
A(29-28-33)	122.7	119.7
A(28-29-34)	118.7	117.9
A(28-33-32)	121.4	120.0
A(28-33-45)	119.0	120.0
A(29-34-35)	114.6	110.9
A(29-34-46)	110.7	109.9
A(29-34-47)	108.4	108.2
A(31-30-42)	120.7	120.0
A(30-31-32)	119.8	119.9
A(30-31-43)	120.4	120.0
A(32-31-43)	119.8	120.0
A(31-32-33)	120.9	120.1
A(31-32-44)	119.4	119.8
A(33-32-44)	119.7	120.1
A(32-33-45)	119.6	120.0
A(35-34-46)	111.1	109.7
A(35-34-47)	106.2	108.4
A(34-35-36)	110.1	108.4
A(46-34-47)	105.3	109.6
A(35-36-49)	110.6	109.8
A(35-36-50)	113.1	109.6
A(35-36-51)	109.6	109.3
A(49-36-50)	107.9	109.3
A(49-36-51)	107.5	109.4
A(50-36-51)	107.9	109.4

^aAtom label refers to Fig. 3