

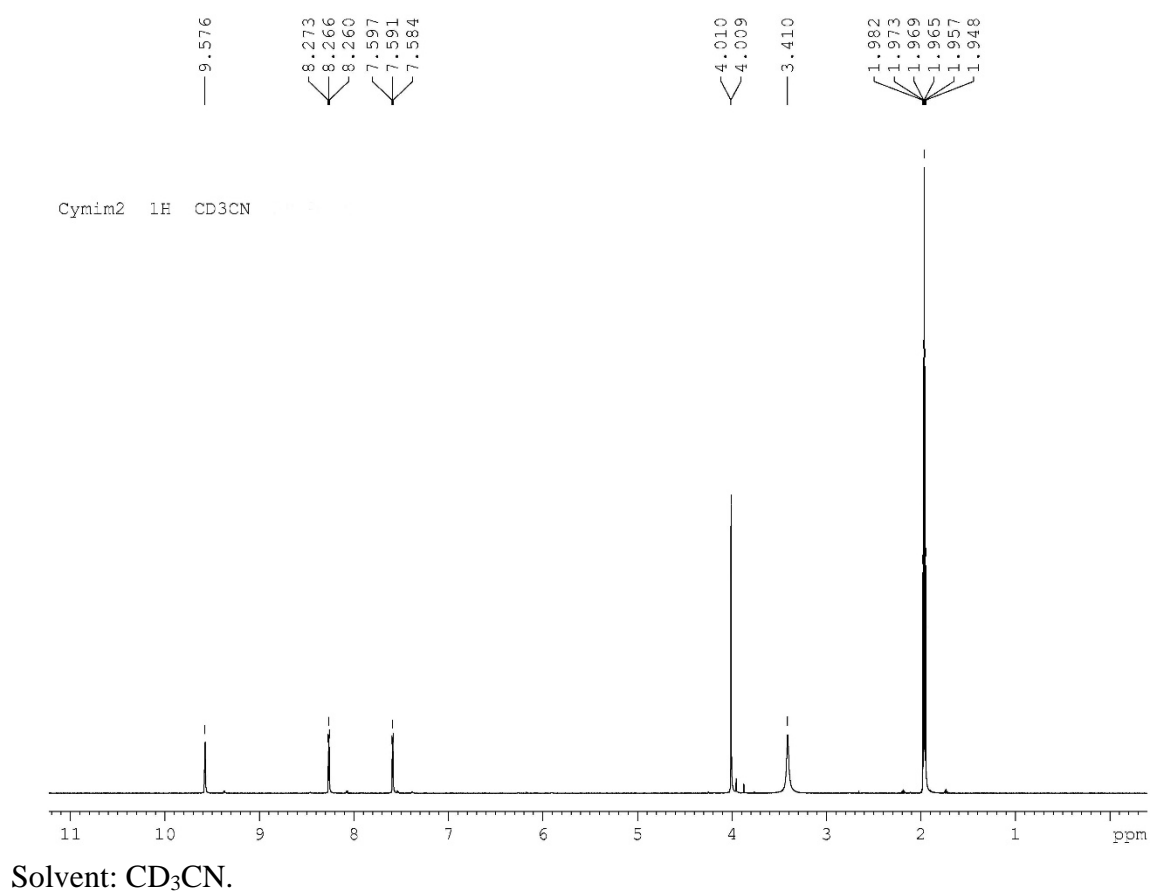
# Novel Triazine-Functionalized Tetra-Imidazolium Hexafluorophosphate Salt: Synthesis, Crystal Structure and DFT study

Abbas W. Salman<sup>1\*</sup>, Rosenani A. Haque<sup>2</sup>, Mustafa M. Kadhim<sup>3</sup>, Frederick P. Malan<sup>4</sup>,  
Ponnadurai Ramasami<sup>5,6\*</sup>

## Supporting Information

1. **Figure SI1:** <sup>1</sup>H-NMR spectrum of compound **4**.
2. **Table SI1:** Atom numbering, bond length and bond angle of compound **4** optimized in the gas phase.

### 1. <sup>1</sup>H-NMR (400 MHz) spectrum of compound **4**.



**2. Table SII:** Atom numbering, bond length and bond angle of compound **4** optimized in the gas phase.

Table SII: Atom numbering, bond length and bond angle of compound <b>4</b> optimized in the gas phase					
Bond length (Å)					
R(1-7)	1.268	R(10-39)	1.479	R(9-11)	1.401
R(1-38)	1.311	R(11-12)	1.360	R(10-12)	1.402
R(2-3)	1.351	R(11-41)	1.072	R(18-46)	1.087
R(2-4)	1.353	R(12-42)	1.073	R(18-47)	1.085
R(3-5)	1.317	R(13-14)	1.357	R(18-48)	1.087
R(3-9)	1.431	R(13-15)	1.401	R(19-25)	1.284
R(4-6)	1.315	R(14-16)	1.339	R(19-38)	1.122
R(4-13)	1.431	R(14-43)	1.071	R(20-21)	1.353
R(5-7)	1.392	R(15-17)	1.360	R(20-22)	1.349
R(6-7)	1.391	R(15-44)	1.072	R(21-23)	1.319
R(8-9)	1.357	R(16-17)	1.402	R(21-27)	1.426
R(8-10)	1.339	R(16-18)	1.479	R(22-24)	1.321
R(8-40)	1.071	R(17-45)	1.073	R(22-31)	1.426

R(23-25)	1.379	R(30-51)	1.073	R(36-55)	1.087
R(24-25)	1.378	R(31-32)	1.359	R(36-56)	1.085
R(26-27)	1.359	R(31-33)	1.402	R(36-57)	1.087
R(26-28)	1.338	R(32-34)	1.338	R(37-58)	1.087
R(26-49)	1.071	R(32-52)	1.071	R(37-59)	1.085
R(27-29)	1.403	R(33-35)	1.359	R(37-60)	1.087
R(28-30)	1.403	R(33-53)	1.072	R(39-61)	1.087
R(28-37)	1.480	R(34-35)	1.403	R(39-62)	1.087
R(29-30)	1.359	R(34-36)	1.480	R(39-63)	1.085
R(29-50)	1.072	R(35-54)	1.073		
Bond Angle (°)					
A(7-1-38)	126.8	A(4-13-15)	124.7	A(12-11-41)	132.7
A(1-7-5)	121.1	A(5-7-6)	119.4	A(11-12-42)	130.8
A(1-7-6)	119.5	A(9-8-10)	107.9	A(14-13-15)	109.1
A(1-38-19)	179.4	A(9-8-40)	125.1	A(13-14-16)	107.9
A(3-2-4)	111.4	A(8-9-11)	109.1	A(13-14-43)	125.1
A(2-3-5)	127.9	A(10-8-40)	127.0	A(13-15-17)	106.6
A(2-3-9)	116.1	A(8-10-12)	109.0	A(13-15-44)	120.7
A(2-4-6)	128.0	A(8-10-39)	126.1	A(16-14-43)	127.0
A(2-4-13)	116.1	A(9-11-12)	106.6	A(14-16-17)	109.0
A(5-3-9)	116.0	A(9-11-41)	120.7	A(14-16-18)	126.1
A(3-5-7)	116.7	A(12-10-39)	124.9	A(17-15-44)	132.7
A(3-9-8)	126.1	A(10-12-11)	107.4	A(15-17-16)	107.4
A(3-9-11)	124.8	A(10-12-42)	121.8	A(15-17-45)	130.8
A(6-4-13)	115.9	A(10-39-61)	109.5	A(17-16-18)	124.9
A(4-6-7)	116.6	A(10-39-62)	109.5	A(16-17-45)	121.8
A(4-13-14)	126.2	A(10-39-63)	109.3	A(16-18-46)	109.5
A(16-18-47)	109.2	A(23-25-24)	120.6	A(31-33-53)	120.8

A(16-18-48)	109.5	A(27-26-28)	107.9	A(34-32-52)	127.0
A(46-18-47)	109.3	A(27-26-49)	125.2	A(32-34-35)	109.1
A(46-18-48)	110.0	A(26-27-29)	109.0	A(32-34-36)	126.1
A(47-18-48)	109.3	A(28-26-49)	126.9	A(35-33-53)	132.7
A(25-19-38)	122.8	A(26-28-30)	109.1	A(33-35-34)	107.5
A(19-25-23)	118.2	A(26-28-37)	126.1	A(33-35-54)	130.8
A(19-25-24)	121.1	A(27-29-30)	106.6	A(35-34-36)	124.8
A(21-20-22)	111.8	A(27-29-50)	120.9	A(34-35-54)	121.8
A(20-21-23)	127.6	A(30-28-37)	124.8	A(34-36-55)	109.4
A(20-21-27)	116.5	A(28-30-29)	107.5	A(34-36-56)	109.3
A(20-22-24)	127.5	A(28-30-51)	121.8	A(34-36-57)	109.4
A(20-22-31)	116.7	A(28-37-58)	109.4	A(55-36-56)	109.4
A(23-21-27)	115.9	A(28-37-59)	109.3	A(55-36-57)	110.0
A(21-23-25)	116.2	A(28-37-60)	109.4	A(56-36-57)	109.4
A(21-27-26)	126.3	A(30-29-50)	132.6	A(58-37-59)	109.4
A(21-27-29)	124.7	A(29-30-51)	130.7	A(58-37-60)	110.0
A(24-22-31)	115.9	A(32-31-33)	109.1	A(59-37-60)	109.4
A(22-24-25)	116.3	A(31-32-34)	107.8	A(61-39-62)	110.0
A(22-31-32)	126.2	A(31-32-52)	125.2	A(61-39-63)	109.3
A(22-31-33)	124.7	A(31-33-35)	106.5	A(62-39-63)	109.3