Anion directed supramolecular architecture of pyrazole based ionic salts

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Supporting Information

Caption of Figures

Fig. S1 Molecular structure of salt **1** showing various interactions. Color code: C, grey; P, cyan; O, red; N, blue.

Fig. S2 Molecular structure of salt **2** showing various interactions. Color code: C, grey; O, red; N, blue.

Fig. S3 Molecular structure of salt **3** showing various N-H···Cl and C-H···Cl interaction. Color code: C, grey; Cl, green; N, blue.

Fig. S4 Orientation and interaction among pyrazoles in salt **4.**

Fig. S5 Non-covalent interactions of sulphate (pink colored) with pyrazoles in salt **4** (Other molecules are omitted for clarity).

Fig. S6 Non-covalent interactions of bisulphate (yellow colored) with pyrazoles in salt **4** (Other molecules are omitted for clarity).

Fig. S7 Different O-H····O interactions among the sulphate, pink; bisulphate, yellow; water, cyan in salt **4**.

Fig. S8 Different non covalent interaction in salt **5**. Color code: C, grey; Cl, green; O, red; N, blue.

Fig. S9 Different non-covalent interactions among the perchlorate, methanol and water molecule in salt **5.** Color code: C, grey; Cl, green; O, red.

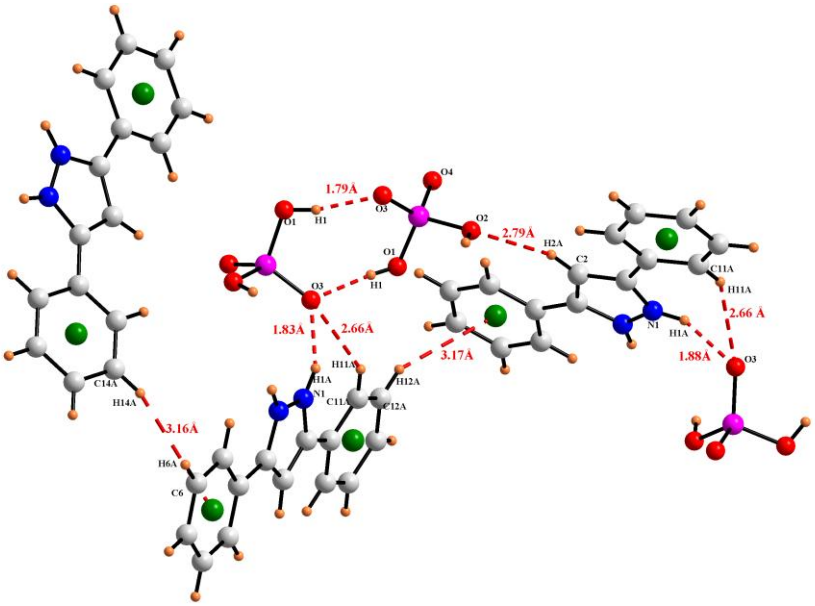

Fig. S1

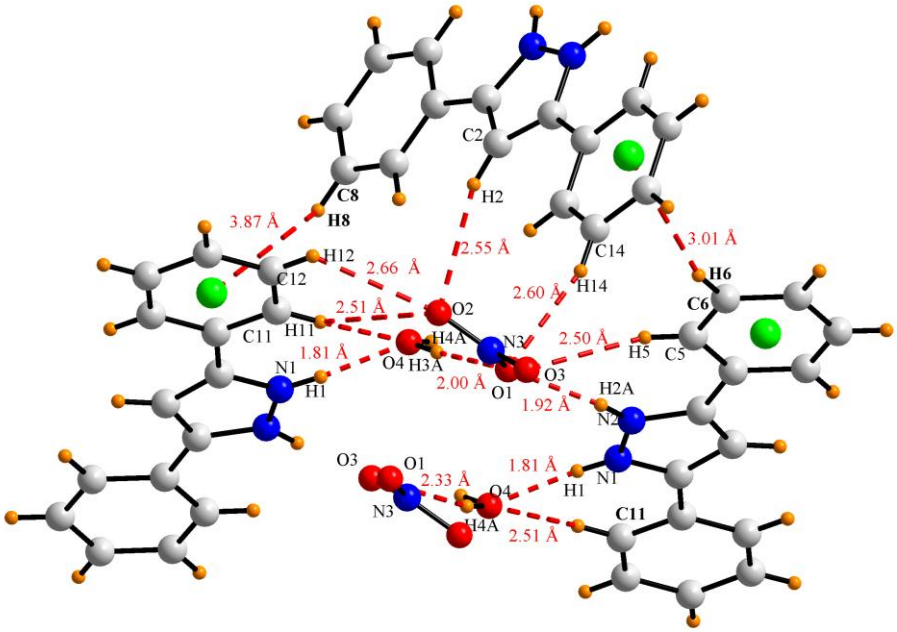

Fig. S2

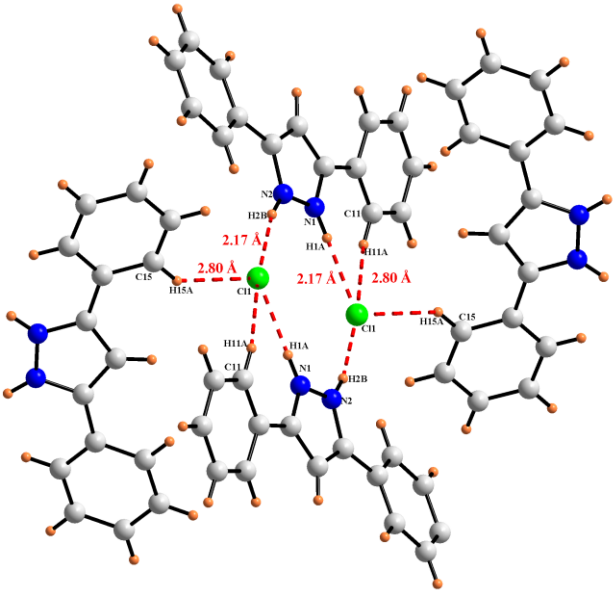

Fig. S3

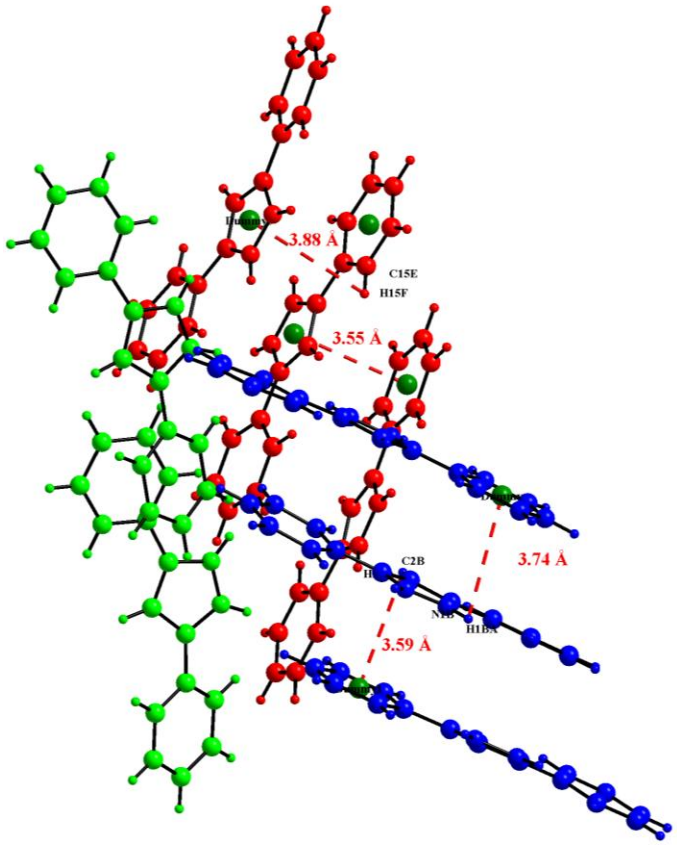

Fig. S4

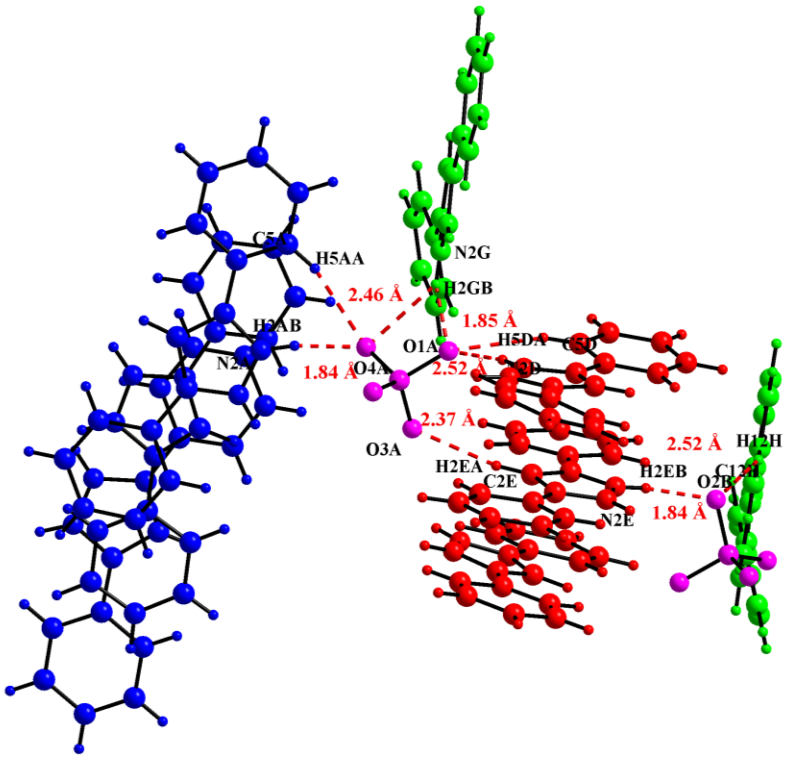

Fig. S5

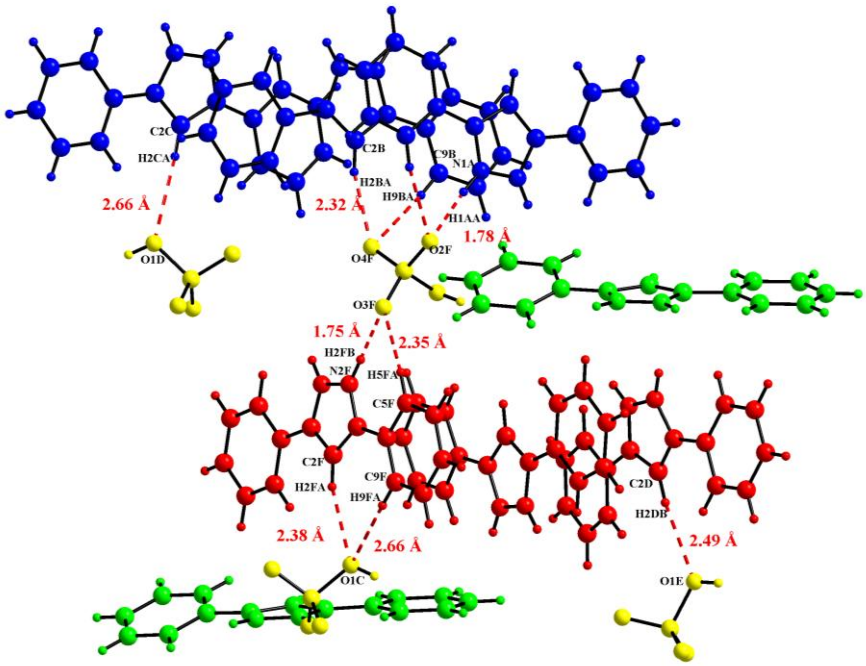

Fig. S6

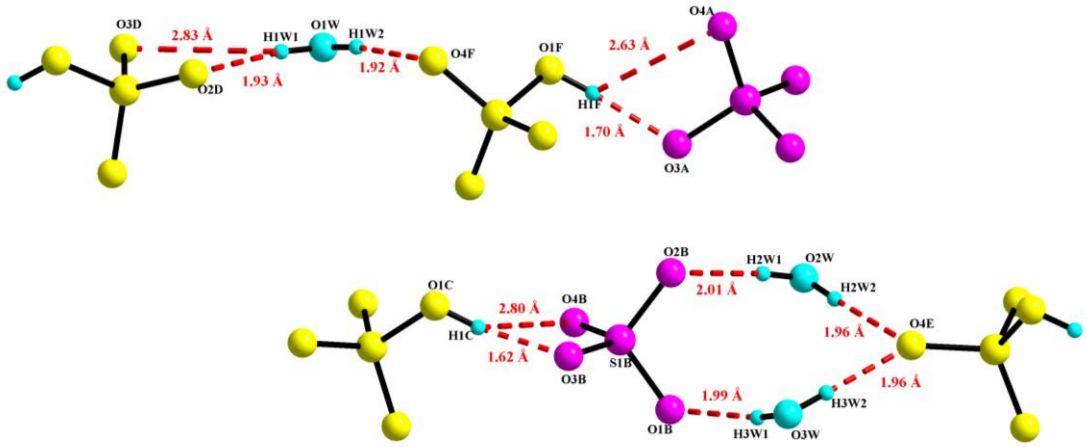

Fig. S7

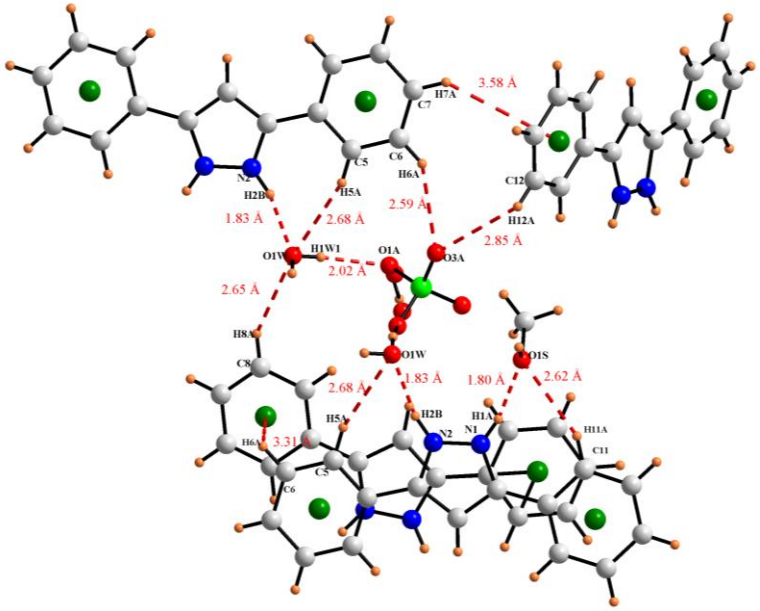

Fig. S8

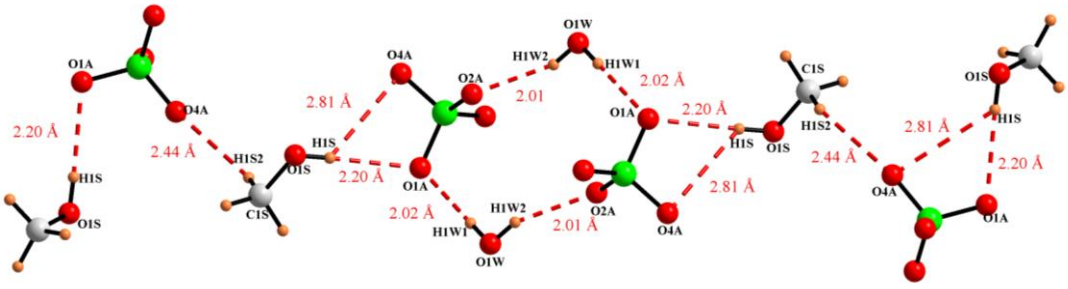

Fig. S9

Table S1 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for salt **1-5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

1.

	x	y	z	U(eq)
P(1)	10192(1)	3885(1)	7845(1)	29(1)
O(1)	10906(1)	4432(1)	8193(4)	48(1)
O(2)	10497(1)	3335(1)	5662(3)	43(1)
O(3)	9416(1)	4252(1)	6862(3)	36(1)
O(4)	10100(1)	3464(1)	10425(2)	38(1)
N(1)	8281(1)	3555(1)	3998(3)	32(1)
N(2)	8572(1)	3133(1)	2017(3)	31(1)
C(1)	7491(1)	3376(1)	4543(4)	31(1)
C(2)	7283(1)	2825(1)	2821(4)	34(1)
C(3)	7974(1)	2682(1)	1254(4)	30(1)
C(4)	8094(1)	2152(1)	-888(4)	33(1)
C(5)	8855(1)	2072(1)	-2172(4)	44(1)
C(6)	8957(2)	1563(1)	-4175(5)	55(1)
C(7)	8297(2)	1139(1)	-4912(5)	55(1)
C(8)	7545(2)	1216(1)	-3660(5)	54(1)
C(9)	7441(1)	1716(1)	-1659(5)	45(1)
C(10A)	6987(5)	3716(6)	6639(17)	33(1)
C(11A)	7276(6)	4325(5)	7910(20)	41(1)
C(12A)	6796(8)	4655(4)	9880(20)	52(1)
C(13A)	6027(7)	4377(6)	10579(17)	62(1)
C(14A)	5738(5)	3768(7)	9310(20)	61(2)
C(15A)	6218(5)	3437(7)	7340(20)	44(2)
C(10B)	7015(11)	3775(11)	6630(40)	33(1)
C(11B)	7375(12)	4285(13)	8290(50)	41(1)
C(12B)	6901(17)	4626(11)	10250(50)	52(1)
C(13B)	6067(16)	4455(11)	10550(40)	62(1)
C(14B)	5707(11)	3945(12)	8900(40)	61(2)
C(15B)	6181(12)	3605(10)	6940(30)	44(2)

2.

	x	y	z	U(eq)
O(1)	1664(1)	4734(1)	5937(1)	27(1)
O(2)	-523(2)	3636(1)	5528(1)	35(1)
O(3)	-1732(2)	4857(1)	6130(1)	35(1)
O(1W)	5179(2)	6211(1)	4955(1)	26(1)
N(1)	4893(2)	6476(1)	6587(1)	20(1)
N(2)	3188(2)	6117(1)	6949(1)	20(1)
N(3)	-229(2)	4406(1)	5863(1)	23(1)
C(1)	5955(2)	7042(1)	7138(1)	19(1)
C(2)	4872(2)	7032(1)	7874(1)	20(1)
C(3)	3130(2)	6442(1)	7738(1)	19(1)
C(4)	1466(2)	6178(1)	8306(1)	20(1)
C(5)	-96(2)	5518(1)	8084(1)	24(1)
C(6)	-1637(2)	5288(1)	8640(1)	27(1)
C(7)	-1647(2)	5717(1)	9417(1)	28(1)
C(8)	-117(2)	6381(1)	9636(1)	30(1)
C(9)	1438(2)	6611(1)	9085(1)	27(1)
C(10)	7889(2)	7548(1)	6931(1)	19(1)
C(11)	8817(2)	7420(1)	6166(1)	24(1)
C(12)	10652(2)	7908(1)	5987(1)	26(1)
C(13)	11579(2)	8520(1)	6573(1)	25(1)
C(14)	10679(2)	8641(1)	7337(1)	26(1)
C(15)	8838(2)	8163(1)	7518(1)	23(1)

3.

	x	y	z	U(eq)
Cl(1)	2795(1)	4409(1)	-389(1)	47(1)
N(1)	5434(1)	3793(1)	2007(1)	38(1)
N(2)	6918(1)	4158(1)	2253(1)	39(1)
C(1)	5480(2)	3159(1)	2858(1)	35(1)

C(2)	7057(2)	3131(1)	3667(1)	41(1)
C(3)	7941(2)	3765(1)	3275(1)	37(1)
C(4)	9650(2)	4006(1)	3829(1)	38(1)
C(5)	10502(2)	4551(1)	3145(2)	48(1)
C(6)	12131(2)	4732(1)	3708(2)	57(1)
C(7)	12908(2)	4374(1)	4955(2)	56(1)
C(8)	12064(2)	3839(1)	5645(2)	58(1)
C(9)	10452(2)	3653(1)	5088(2)	51(1)
C(10)	4063(2)	2636(1)	2897(1)	35(1)
C(11)	2470(2)	2827(1)	2232(1)	41(1)
C(12)	1165(2)	2325(1)	2340(2)	51(1)
C(13)	1432(2)	1636(1)	3116(2)	56(1)
C(14)	3014(2)	1438(1)	3762(2)	57(1)
C(15)	4330(2)	1930(1)	3658(2)	46(1)

4.

	x	y	z	U(eq)
S(1A)	2639(1)	782(1)	2929(1)	18(1)
O(1A)	2284(2)	1208(1)	3414(1)	21(1)
O(2A)	1977(2)	232(1)	2694(1)	34(1)
O(3A)	3559(2)	513(1)	3283(1)	26(1)
O(4A)	2699(2)	1192(1)	2342(1)	22(1)
S(1B)	6065(1)	743(1)	7741(1)	18(1)
O(1B)	5607(2)	283(1)	8131(1)	19(1)
O(2B)	5345(2)	1203(1)	7345(1)	20(1)
O(3B)	6433(2)	343(1)	7246(1)	22(1)
O(4B)	6817(2)	1113(1)	8208(1)	22(1)
S(1C)	8841(1)	493(1)	7493(1)	19(1)
O(1C)	7908(2)	654(2)	6976(1)	30(1)
O(2C)	8692(2)	-43(1)	7930(1)	24(1)
O(3C)	9155(2)	1082(1)	7898(1)	26(1)
O(4C)	9463(2)	311(1)	7067(1)	30(1)
S(1D)	9753(1)	578(1)	2663(1)	19(1)

O(1D)	10338(2)	587(1)	2127(1)	27(1)
O(2D)	8791(2)	569(1)	2272(1)	30(1)
O(3D)	9983(2)	1171(1)	3089(1)	24(1)
O(4D)	10030(2)	-9(1)	3089(1)	23(1)
S(1E)	1747(1)	812(1)	7862(1)	21(1)
O(1E)	1034(2)	858(2)	7143(1)	32(1)
O(2E)	1501(2)	254(1)	8221(1)	28(1)
O(3E)	1673(2)	1434(1)	8217(1)	28(1)
O(4E)	2655(2)	754(1)	7705(1)	32(1)
S(1F)	5333(1)	367(1)	2496(1)	22(1)
O(1F)	4884(2)	950(1)	2801(2)	34(1)
O(2F)	4584(2)	-21(1)	2053(1)	29(1)
O(3F)	5849(2)	-35(1)	3067(1)	29(1)
O(4F)	5946(2)	690(2)	2133(1)	34(1)
O(1W)	7601(2)	1169(1)	2946(1)	27(1)
O(2W)	4171(2)	1588(1)	8194(1)	26(1)
O(3W)	3861(2)	-116(1)	7303(1)	24(1)
N(1A)	3278(2)	345(1)	956(1)	17(1)
N(2A)	2661(2)	801(2)	1044(1)	19(1)
C(1A)	3166(2)	235(2)	281(2)	18(1)
C(2A)	2439(2)	639(2)	-61(2)	18(1)
C(3A)	2130(2)	996(2)	430(2)	19(1)
C(4A)	1396(2)	1504(2)	352(2)	18(1)
C(5A)	1198(3)	1808(2)	917(2)	26(1)
C(6A)	519(3)	2301(2)	829(2)	36(1)
C(7A)	36(3)	2490(2)	167(2)	34(1)
C(8A)	220(3)	2185(2)	-386(2)	34(1)
C(9A)	901(3)	1691(2)	-303(2)	26(1)
C(10A)	3747(2)	-242(2)	20(2)	16(1)
C(11A)	4433(3)	-625(2)	462(2)	25(1)
C(12A)	4982(3)	-1064(2)	198(2)	26(1)
C(13A)	4854(3)	-1118(2)	-501(2)	23(1)
C(14A)	4175(3)	-747(2)	-944(2)	26(1)
C(15A)	3623(3)	-314(2)	-684(2)	22(1)
N(1B)	5711(2)	632(2)	-588(1)	21(1)
N(2B)	5078(2)	1105(1)	-568(1)	20(1)

C(1B)	6162(2)	461(2)	56(2)	22(1)
C(2B)	5785(2)	841(2)	500(2)	22(1)
C(3B)	5101(3)	1242(2)	94(2)	22(1)
C(4B)	4474(3)	1734(2)	280(2)	21(1)
C(5B)	3889(3)	2132(2)	-212(2)	27(1)
C(6B)	3273(3)	2564(2)	-24(2)	29(1)
C(7B)	3239(3)	2614(2)	653(2)	33(1)
C(8B)	3818(3)	2214(2)	1140(2)	31(1)
C(9B)	4443(3)	1790(2)	960(2)	25(1)
C(10B)	6917(3)	-39(2)	195(2)	23(1)
C(11B)	7149(3)	-385(2)	-338(2)	23(1)
C(12B)	7887(3)	-837(2)	-201(2)	31(1)
C(13B)	8398(3)	-941(2)	479(2)	32(1)
C(14B)	8185(3)	-591(2)	1004(2)	35(1)
C(15B)	7439(3)	-143(2)	869(2)	28(1)
N(1C)	8957(2)	430(2)	-770(1)	20(1)
N(2C)	8336(2)	900(1)	-716(1)	19(1)
C(1C)	9533(2)	314(2)	-149(2)	21(1)
C(2C)	9246(2)	718(2)	314(2)	22(1)
C(3C)	8480(2)	1086(2)	-55(2)	19(1)
C(4C)	7917(3)	1583(2)	177(2)	24(1)
C(5C)	7267(3)	1979(2)	-284(2)	26(1)
C(6C)	6730(3)	2438(2)	-47(2)	32(1)
C(7C)	6833(3)	2516(2)	643(2)	41(1)
C(8C)	7466(3)	2125(2)	1112(2)	45(1)
C(9C)	8003(3)	1667(2)	879(2)	34(1)
C(10C)	10296(2)	-182(2)	-48(2)	19(1)
C(11C)	10564(3)	-455(2)	-595(2)	23(1)
C(12C)	11289(3)	-923(2)	-479(2)	29(1)
C(13C)	11745(3)	-1103(2)	178(2)	29(1)
C(14C)	11480(3)	-825(2)	731(2)	29(1)
C(15C)	10753(3)	-369(2)	622(2)	27(1)
N(1D)	852(2)	374(1)	4393(1)	17(1)
N(2D)	1512(2)	849(1)	4487(1)	18(1)
C(1D)	629(2)	256(2)	4993(2)	15(1)
C(2D)	1194(2)	663(2)	5479(2)	19(1)

C(3D)	1739(2)	1038(2)	5154(2)	18(1)
C(4D)	2411(2)	1568(2)	5423(2)	19(1)
C(5D)	2804(3)	1958(2)	4993(2)	25(1)
C(6D)	3401(3)	2475(2)	5264(2)	29(1)
C(7D)	3626(3)	2600(2)	5966(2)	32(1)
C(8D)	3259(3)	2211(2)	6393(2)	31(1)
C(9D)	2651(3)	1696(2)	6125(2)	23(1)
C(10D)	-94(2)	-229(2)	5055(2)	19(1)
C(11D)	-731(2)	-497(2)	4484(2)	21(1)
C(12D)	-1399(3)	-943(2)	4571(2)	25(1)
C(13D)	-1451(3)	-1134(2)	5226(2)	27(1)
C(14D)	-823(3)	-864(2)	5787(2)	27(1)
C(15D)	-143(3)	-419(2)	5714(2)	26(1)
N(1E)	3989(2)	259(1)	6046(1)	18(1)
N(2E)	4607(2)	749(2)	6061(1)	17(1)
C(1E)	3654(2)	56(2)	5386(2)	17(1)
C(2E)	4075(2)	435(2)	4984(2)	18(1)
C(3E)	4685(2)	867(2)	5421(2)	18(1)
C(4E)	5332(2)	1374(2)	5274(2)	18(1)
C(5E)	5868(3)	1777(2)	5783(2)	26(1)
C(6E)	6477(3)	2230(2)	5634(2)	33(1)
C(7E)	6560(3)	2287(2)	4967(2)	32(1)
C(8E)	6037(3)	1898(2)	4455(2)	28(1)
C(9E)	5412(3)	1442(2)	4598(2)	23(1)
C(10E)	2942(2)	-473(2)	5201(2)	17(1)
C(11E)	2567(3)	-784(2)	5690(2)	22(1)
C(12E)	1885(3)	-1270(2)	5490(2)	25(1)
C(13E)	1572(3)	-1449(2)	4814(2)	28(1)
C(14E)	1947(3)	-1152(2)	4326(2)	27(1)
C(15E)	2631(3)	-660(2)	4513(2)	23(1)
N(1F)	7650(2)	804(2)	4226(1)	20(1)
N(2F)	6996(2)	347(2)	4231(1)	21(1)
C(1F)	8104(2)	951(2)	4880(2)	19(1)
C(2F)	7714(2)	570(2)	5302(2)	22(1)
C(3F)	7010(2)	190(2)	4882(2)	19(1)
C(4F)	6361(2)	-300(2)	5055(2)	19(1)

C(5F)	5721(3)	-655(2)	4540(2)	23(1)
C(6F)	5118(3)	-1104(2)	4725(2)	28(1)
C(7F)	5147(3)	-1215(2)	5406(2)	25(1)
C(8F)	5777(3)	-859(2)	5913(2)	29(1)
C(9F)	6377(3)	-408(2)	5736(2)	27(1)
C(10F)	8872(2)	1436(2)	5048(2)	20(1)
C(11F)	9231(3)	1729(2)	4544(2)	28(1)
C(12F)	9952(3)	2175(2)	4723(2)	28(1)
C(13F)	10336(3)	2344(2)	5396(2)	26(1)
C(14F)	9992(3)	2047(2)	5903(2)	27(1)
C(15F)	9262(3)	1601(2)	5735(2)	25(1)
N(1H)	9551(2)	2341(2)	7723(1)	22(1)
N(2H)	10469(2)	2404(1)	7761(1)	22(1)
C(1H)	9131(3)	2940(2)	7581(2)	21(1)
C(2H)	9823(3)	3388(2)	7520(2)	22(1)
C(3H)	10669(3)	3036(2)	7645(2)	20(1)
C(4H)	11610(3)	3263(2)	7657(2)	21(1)
C(5H)	12416(3)	2910(2)	8000(2)	30(1)
C(6H)	13302(3)	3161(2)	8027(2)	31(1)
C(7H)	13397(3)	3764(2)	7712(2)	29(1)
C(8H)	12597(3)	4107(2)	7375(2)	31(1)
C(9H)	11712(3)	3863(2)	7353(2)	28(1)
C(10H)	8129(3)	3041(2)	7519(2)	20(1)
C(11H)	7531(3)	2533(2)	7612(2)	31(1)
C(12H)	6589(3)	2649(2)	7566(2)	34(1)
C(13H)	6233(3)	3292(2)	7427(2)	33(1)
C(14H)	6813(3)	3806(2)	7338(2)	29(1)
C(15H)	7760(3)	3680(2)	7385(2)	26(1)
N(1G)	645(2)	2355(1)	2856(1)	18(1)
N(2G)	1548(2)	2344(1)	2849(1)	20(1)
C(1G)	288(3)	2965(2)	2679(2)	18(1)
C(2G)	1016(2)	3352(2)	2566(2)	18(1)
C(3G)	1809(3)	2947(2)	2681(2)	19(1)
C(4G)	2772(2)	3080(2)	2645(2)	17(1)
C(5G)	3513(3)	2668(2)	2962(2)	25(1)
C(6G)	4418(3)	2793(2)	2908(2)	30(1)

C(7G)	4580(3)	3341(2)	2536(2)	28(1)
C(8G)	3852(3)	3765(2)	2224(2)	24(1)
C(9G)	2954(3)	3638(2)	2282(2)	22(1)
C(10G)	-685(2)	3124(2)	2664(2)	18(1)
C(11G)	-1286(2)	2659(2)	2843(2)	21(1)
C(12G)	-2192(3)	2819(2)	2840(2)	25(1)
C(13G)	-2525(3)	3456(2)	2647(2)	27(1)
C(14G)	-1955(3)	3923(2)	2462(2)	30(1)
C(15G)	-1032(3)	3759(2)	2472(2)	25(1)

5.

	x	y	z	U(eq)
Cl(1)	4752(1)	-873(1)	3831(1)	38(1)
O(1A)	4541(3)	-2386(4)	4031(2)	51(2)
O(2A)	5306(2)	-284(5)	4197(2)	64(2)
O(3A)	4155(2)	156(6)	3846(3)	114(4)
O(4A)	5012(4)	-995(8)	3248(2)	132(4)
O(1B)	4671(4)	-2510(4)	3930(3)	40(3)
O(2B)	4253(3)	-373(9)	3401(3)	64(3)
O(3B)	4621(5)	-45(8)	4361(2)	91(5)
O(4B)	5460(2)	-555(10)	3637(4)	92(5)
O(1S)	5398(2)	5050(4)	3382(2)	49(1)
O(1W)	5543(2)	2661(4)	4719(1)	33(1)
N(1)	6747(2)	4246(3)	3695(1)	23(1)
N(2)	6806(2)	3302(3)	4171(1)	23(1)
C(1)	7410(2)	4523(4)	3469(2)	23(1)
C(2)	7906(2)	3722(4)	3826(1)	22(1)
C(3)	7511(2)	2962(4)	4267(1)	21(1)
C(4)	7761(2)	1982(4)	4764(1)	21(1)
C(5)	7275(2)	1125(4)	5117(2)	23(1)
C(6)	7529(2)	229(4)	5588(2)	25(1)
C(7)	8270(2)	168(5)	5708(2)	28(1)
C(8)	8751(2)	1009(5)	5358(2)	29(1)

C(9)	8501(2)	1916(4)	4888(2)	26(1)
C(10)	7538(2)	5502(4)	2941(2)	23(1)
C(11)	6964(2)	6011(4)	2578(2)	29(1)
C(12)	7112(2)	6935(5)	2082(2)	34(1)
C(13)	7820(2)	7356(5)	1948(2)	33(1)
C(14)	8383(2)	6854(5)	2304(2)	32(1)
C(15)	8246(2)	5929(4)	2798(2)	28(1)
C(1S)	4904(3)	3827(8)	3192(3)	60(2)

Table S2 Comparison of bond lengths (Å) and bond angles (^{o}) in solid and gaseous phase for the salts **1-5**

Parameters	X-ray	B3LYP/6-31G(d,p)
$Pz^{Ph2}H_2^+$-$H_2PO_4^-$ (1)		
Bond Length		
P1-O1	1.556(18)	1.676
P1-O2	1.574(19)	1.648
P1-O3	1.511(17)	1.495
P1-O4	1.507(17)	1.514
O1-H1A	0.700(3)	0.966
O2-H2A	0.790(5)	0.966
N1-N2	1.347(3)	1.381
N1-C9	1.341(3)	1.372
N1-H1B	0.860	1.012
N2-C7	1.346(3)	1.369
N2-H2B	0.8600	1.011
C1-C2	1.381(4)	1.389
C1-C6	1.391(4)	1.408
C1-H1	0.930	1.087
C2-C3	1.381(5)	1.399
C3-C4	1.363(6)	1.395
C4-C5	1.393(5)	1.393
C5-C6	1.399(4)	1.408
C6-C7	1.465(3)	1.457
C7-C8	1.390(3)	1.399
C8-C9	1.385(3)	1.392
C9-C10	1.469(3)	1.458
C10- C11	1.388(4)	1.407
C10-C15	1.393(3)	1.407
C11-C12	1.388(4)	1.390

C13-C14	1.372(5)	1.396
C12-C13	1.378(5)	1.398
Angle		
O1-P1-O2	106.3(13)	102.3
O4-P1-O1	109.2(12)	104.6
P1-O1-H1A	110(3)	105.7
P1-O2-H2A	109(4)	106.0
O1-P1-H1A	20.1(11)	25.6
O2-P1-H1A	113.2(12)	105.5
O3-P1-O1	110.11(10)	107.7
O3-P1-H1A	90.1(11)	82.8
O3-P1-O2	109.93(11)	109.3
O4-P1-O3	115.5(11)	123.7
O4-P1-H1A	122.2(12)	125.7
O4-P1-O2	105.2(11)	104.6
C9-N1-N2	109.1(19)	107.8
C9-N1-H1B	125.4	122.7
N2-N1-H1B	125.4	116.7
C7-N2-H2B	125.5	123.8
C7-N2-N1	109.1(19)	108.3
N1-N2-H2B	125.5	117.1
C4-C5-H5	120.3	120.0
C2-C1-C6	120.7(3)	120.2
C1-C2-C3	120.0(3)	119.8
C4-C3-C2	120.0(3)	120.1
C1-C6-C7	121.6(2)	121.3
C3-C4-C5	121.1(3)	120.7
C4-C5-C6	119.3(3)	119.2
N2-C7-C8	107.3(2)	107.8
C5-C6-C7	119.4(2)	118.8
N2-C7-C6	122.6(2)	122.5
$Pz^{Ph2}H_2^+$-NO_3^- (2)		
Bond Length		
O1-N3	1.273 (15)	1.224
O2-N3	1.241(16)	1.211
O3-N3	1.237(17)	1.376
N1-N2	1.345(16)	1.349
N1-C1	1.346(17)	1.360
N1-H1	0.860	1.009
N2-C3	1.346(18)	1.342
N2-H2A	0.860	1.685
C1-C2	1.390(18)	1.388

C2-C3	1.388(18)	1.415
C2-H2	0.930	1.078
C1-C10	1.465(18)	1.466
C3-C4	1.470(18)	1.471
C4-C9	1.392(2)	1.463
C1- C13	1.385(2)	1.395
C4-C5	1.395(2)	1.404
C6-H6	0.930	1.086
C5-C6	1.387(2)	1.393
C6-C7	1.387(2)	1.396
C1- C14	1.387(2)	1.396
C7-C8	1.385(2)	1.395
C8-C9	1.389(2)	1.393
C9-H9	0.930	1.085
C10-C11	1.395(19)	1.404
C10-C15	1.396(19)	1.404
C11-C12	1.389(2)	1.086
Angle		
N2-N1-C1	109.0(11)	113.0
N1-C1-C10	122.4(12)	122.8
N2-N1-H1	125.5	119.0
N1-N2-C3	109.4(11)	105.5
N1-C1-C2	107.3(12)	105.3
N1-N2-H2A	125.3	112.8
O3-N3-O2	121.4(13)	127.9
O2-N3-O1	119.0(13)	114.7
O3-N3-O1	119.6(12)	117.2
C2-C1-C10	130.1(12)	131.8
N2-C3-C2	107.1(12)	109.8
C3-C2-C1	106.9(12)	106.2
C9-C4-C3	118.8(12)	120.1
C2-C3-C4	129.6(12)	128.2
N2-C3-C4	123.1(12)	121.9
C9-C4-C5	119.1(13)	118.9
C5-C4-C3	121.9(12)	120.9
C6-C5-C4	120.2(13)	120.2
C5-C6-C7	120.2(14)	120.4
C7-C8-C9	120.2(14)	120.1
C8-C7-C6	119.7(14)	119.6
C8-C9-C4	120.3(14)	120.6
C11-C10-C15	119.1(13)	118.8
C11-C10-C1	121.5(12)	121.1
C15-C10-C1	119.2(12)	120.0

C12-C11-C10	120.2(13)	120.5
$Pz^{Ph2}H_2^+$-Cl^- (3)		
Bond Length		
N1-N2	1.350(17)	1.382
N1-H1A	0.930(2)	1.012
C7-N1	1.341(19)	1.371
C3-C2	1.380(2)	1.393
C4-C5	1.390(2)	1.407
C4-C3	1.396(2)	1.409
C4-C7	1.466(2)	1.457
C9-N2	1.343(18)	1.371
C9-C8	1.383(2)	1.393
C9-C10	1.467(19)	1.457
C7-C8	1.388(2)	1.393
C10-C15	1.383(2)	1.407
C10-C11	1.393(2)	1.409
C6-C1	1.378(3)	1.398
C14-C13	1.379(3)	1.398
C5 -6	1.383(2)	1.389
C3-H3	0.930	1.092
C5-H5	0.930	0.980
C8-H8	0.930	1.108
C15-C14	1.389(2)	1.389
C15-H15	0.930	1.087
C6- H6	0.930	1.085
C11-C12	1.376(2)	1.393
C2-C1	1.379(3)	1.395
C13-C12	1.367(3)	1.395
Angle		
C5-C4-C3	119.1(14)	119.8
C5-C4-C7	122.2(13)	121.8
C3-C4-C7	118.5(13)	118.3
N2-C9-C8	106.7(13)	108.0
N2-C9-C10	124.1(13)	123.3
N1-C7-C8	106.7(13)	108.0
N1-C7-C4	123.9(12)	123.3
C8-C9-C10	129.1(13)	128.6
C8-C7-C4	129.3(13)	128.6
C15-C10-C11	119.0(14)	119.7
C15-C10-C9	122.9(13)	121.8

C11-C10-C9	118.0(13	118.3
C6-C5-C4	119.9(15)	120.2
C2-C3-C4	120.0(16)	119.3
C9-C8-C7	107.8(12)	107.1
C10-C15-C14	119.6(15)	120.2
C1-C6-C5	120.6(16)	119.8
$Pz^{Ph2}H_2^+$-HSO_4^- (4)		
Bond Length		
S1F O1F	1.549(3)	1.736
S1F O2F	1.457(3)	1.515
S1F O3F	1.453(2)	1.459
S1F O4F	1.451(3)	1.458
O1F H1F	0.8400	0.970
N1A N2A	1.337(4)	1.345
N1A C1A	1.343(4)	1.344
N1A H1AA	0.8800	0.098
N2A C3A	1.341(4)	1.364
N2A H2AB	0.8800	1.033
C1A C2A	1.383(5)	1.406
C2A C3A	1.388(5)	1.398
C1A C10A	1.470(5)	1.467
C3A C4A	1.469(5)	1.466
C4A C5A	1.384(5)	1.405
C4A C9A	1.386(5)	1.403
C5A C6A	1.390(5)	1.392
C6A C7A	1.394(5)	1.396
C7A C8A	1.356(5)	1.396
C8A C9A	1.393(5)	1.396
C10A C15A	1.387(5)	1.405
C10A C11A	1.397(5)	1.403
C11A C12A	1.391(5)	1.392
C12A C13A	1.374(5)	1.396
C13A C14A	1.380(5)	1.396
C14A C15A	1.383(5)	1.392
Angle		
S1F O1F H1F	109.5	105.17
O2F S1F O1F	108.46(15)	101.2
O3F S1F O1F	107.51(16)	103.2
O3F S1F O2F	110.19(16)	113.0
O4F S1F O1F	104.02(16)	101.9
O4F S1F O2F	113.85(15)	113.4
O4F S1F O3F	112.37(15)	12.4

N1A N2A H2AB	125.2	115.1
N1A N2A C3A	109.6(3)	110.3
N1A C1A C2A	106.6(3)	107.2
N1A C1A C10A	122.4(3)	122.2
N2A N1A C1A	109.6(3)	109.0
N2A N1A H1AA	125.2	115.0
C1A C2A C3A	107.7(3)	106.9
C1A N1A H1AA	125.2	125.7
C2A C1A C10A	131.0(3)	130.7
C3A N2A H2AB	125.2	123.4
N2A C3A C2A	106.5(3)	106.4
N2A C3A C4A	122.9(3)	122.2
C2A C3A C4A	130.5(3)	131.2
C5A C4A C9A	119.3(3)	119.2
C5A C4A C3A	121.5(3)	120.7
C9A C4A C3A	119.1(3)	119.9
C4A C5A C6A	120.5(3)	120.1
C5A C6A C7A	119.6(4)	120.2
C8A C7A C6A	119.8(4)	119.8
C7A C8A C9A	121.0(4)	120.1
C4A C9A C8A	119.8(4)	120.3
C15A C10A C11A	118.5(3)	119.2
C15A C10A C1A	119.6(3)	120.7
C11A C10A C1A	121.8(3)	119.4
C12A C11A C10A	120.3(3)	120.3
C13A C12A C11A	119.9(3)	120.1
C12A C13A C14A	120.4(3)	119.8
C13A C14A C15A	119.8(3)	120.3
C14A C15A C10A	121.0(3)	120.0
$Pz^{Ph2}H_2^+$-ClO_4^- (5)		
Bond Length		
Cl1-O1	1.428(4)	1.530
Cl1-O2	1.320(6)	1.530
Cl1-O3	1.264(6)	1.479
Cl1-O4	1.459(8)	1.468
N1-N2	1.337(5)	1.345
N1-C1	1.350(5)	1.346
N1-H1A	1.010(6)	1.050
N2-C9	1.345(5)	1.346
N2-H2A	0.780(4)	1.466
C1-C2	1.480(6)	1.402

C1-C8	1.380(6)	1.403
C2-C3	1.382(6)	1.405
C2-C7	1.401(6)	1.392
C3-C4	1.393(6)	1.396
C4-C5	1.380(6)	1.396
C5-C6	1.390(6)	1.392
C6-C7	1.387(6)	1.392
C8-C9	1.389(6)	1.402
C8-H8	0.930	1.077
C9-C10	1.469(6)	1.466
C10-C11	1.386(6)	1.403
C10-C15	1.393(6)	1.405
C11-C12	1.374(6)	1.396
C13-C14	1.378(7)	1.396
C14-C15	1.388(6)	1.392
Angle		
O1-Cl1-O4	101.9(5)	109.2
O2-Cl1-O4	96.1(7)	109.2
O3-Cl1-O2	128.1(5)	109.1
O3-Cl1-O1	114.4(4)	109.0
O2-Cl1-O1	111.0(4)	106.7
O3-Cl1-O4	97.9(8)	113.1
N2-N1-C1	108.7(3)	109.7
N1-N2-C9	110.1(4)	109.7
N2-N1-H1A	128.0(4)	115.1
C1-N1-H1A	123.0(4)	135.0
N1-C1-C8	107.3(4)	106.6
N1-C1-C2	122.7(4)	122.1
C8-C1-C2	130.0(4)	131.1
C3-C2-C7	119.9(4)	119.2
C3-C2-C1	118.8(4)	119.9
C7-C2-C1	121.3(4)	120.8
C2-C3-C4	120.1(4)	120.3
C5-C4-C3	120.1(4)	120.1
C4-C5-C6	120.2(4)	119.8
C6-C7-C2	119.7(4)	120.2

Table S3 Comparison of energy in gaseous and solid phase in (Kcal/mol)

	Energy of the optimized structure (Gaseous Phase) (Kcal/mol)	**Energy of the optimized structure derived from the solid state (Solid Phase) (Kcal/mol)**
$Pz^{Ph2}H_2^+$-$H_2PO_4^-$ (1)		
	1332.45	1332.47
$Pz^{Ph2}H_2^+$-NO_3^- (2)		
	969.24	969.21
$Pz^{Ph2}H_2^+$-Cl^- (3)		
	1149.11	1149.15
$Pz^{Ph2}H_2^+$-HSO_4^- (4)		
	1388.58	1388.53
$Pz^{Ph2}H_2^+$-ClO_4^- (5)		
	1449.68	1449.63