

## SUPPLEMENTARY MATERIALS

### CHARGES ANALYSIS

The Mülliken charges, obtained at the HF/6-31G\*(6-311++G\*\*) level, shows that the P-N bond is strongly polarized towards the nitrogen atom. The NBO analysis consolidates this tendency with a complete displacement of an electron of phosphorus towards nitrogen. The substitution effect of H by F and OH in  $H_3PNH$  at the HF/6-31G\* level, involves a modification of the charge carried by the nitrogen atom, which causes an evident increase in the dipole moment of  $H_3PNF$  (5.55 Debye) against 3.73 D for  $H_3PNH$  and 3.75 D for  $H_3PNOH$ . The same conclusions are observed when we proceed to the same substitutions in the  $F_3PNH$ . The passage of  $H_3PNX$  to the  $F_3PNX$  one decreases the electronic density of the phosphorus atom to the detriment of the fluorine ones more than on the nitrogen atom, thus decreasing, in all cases, the dipole moment of more than half. The charges NBO analysis leads to the same observations with a multiplication by 1.5 of all the charges.

The complexation effect of  $H_3PNX$  and  $F_3PNX$  by the  $Na^+$  cation, does not lead, in the case of  $H_3PNX$  to a strong modification of the phosphorus charge, on the other hand, in the case of  $F_3PNX$ , the charges of P increases about 6.8 to 8.3 % and that of N of 19.4 to 44.4 %.

It is important to point out that in this case which the nitrogen atom acquires a more significant negative charge when it is connected to the  $Na^+$  cation. The NBO charges lead to the same conclusions with a clear increase in the charge of P and N in comparison to the Mülliken charges. In addition, the HF/6-311++G\*\* calculations obtained for some complexes, lead to the same conclusions with a reduction in the charge of P and an increase in that of N. On the other hand, the effect of the  $Na^+$  cation, multiplies by 2.5 to 3.7 the value of the dipole moment of  $H_3PNX... Na^+$  and about 5.8 to 15.1 that of  $F_3PNX... Na^+$ .