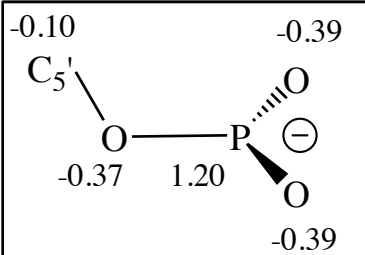
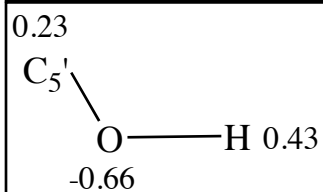


SCAL

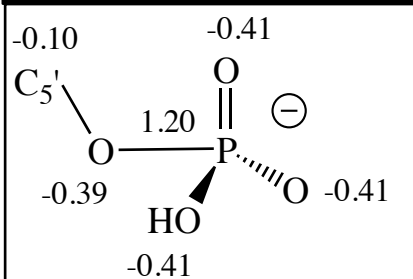
$$R_{010} = -0.05$$



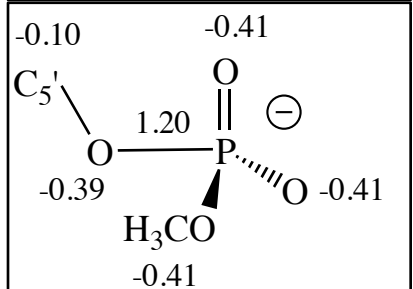
$$R_{110} = 0.00$$



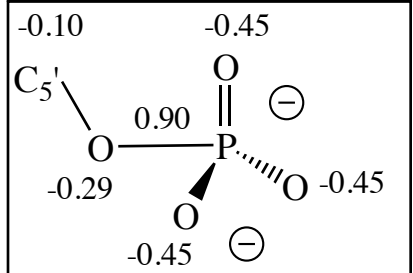
$$R_{210} = -0.32$$



$$R_{310} = -0.32$$

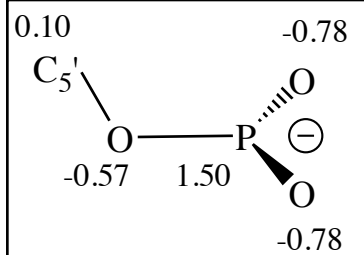


$$R_{410} = -0.64$$

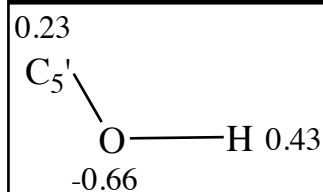


STD,FULL

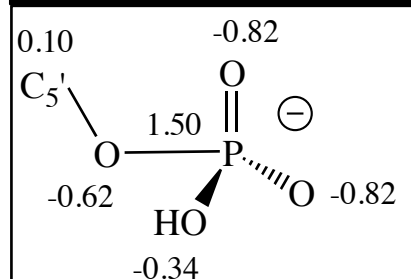
$$R_{010} = -0.53$$



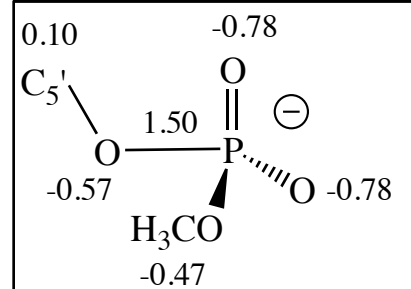
$$R_{110} = 0.00$$



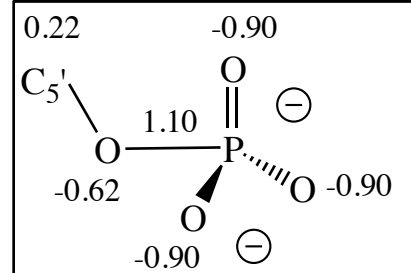
$$R_{210} = -1.00$$



$$R_{310} = -1.00$$



$$R_{410} = -2.00$$



FULL

$$E_{el} = \sum_{excl(i,j)=1}^{\epsilon=1} \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}$$

SCAL, STD

$$E_{el} = \sum_{excl(i,j)=1}^{\epsilon=3} \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}^2} sw(r_{ij}^2, r_{on}^2, r_{off}^2)$$

SCAL, STD, FULL

$$E_{vdw} = \sum_{excl(i,j)=1} \left(\frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^6} \right) sw(r_{ij}^2, r_{on}^2, r_{off}^2)$$