The Potential Corrosion Inhibition Properties of Acetyl Benzoic Acid Derivatives with substituted Alkali metals (Na, K, Li): DFT Approach

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Input File for NEP opt b3lyp/6-311g(d,p) geom=connectivity

3ABA X Y Z	3ABA - Li X Y Z
3ABA/ SCF: -572.796932736 a.u	**3ABA-Li / SCF: -580.444230554 a.u**
O 1.76432 -0.48644 0.	**O 2.23524 1.99509 0.**
O 5.18623 4.39439 0.	**O -3.5716 -0.28331 0.**
O 3.34983 2.8928 0.	**O -2.57525 1.73627 0.**
C 4.19352 -0.432 0.	**C 1.24117 -0.14901 0.**
C 4.37102 0.79773 0.	**C 0. 0.50158 0.**
C 5.46999 1.59135 0.	**C -1.19454 -0.23222 0.**
C 5.42192 -1.11444 0.	**C 1.25682 -1.55643 0.**
C 6.55562 1.05685 0.	**C -1.16325 -1.63248 0.**
C 6.51305 -0.43593 0.	**C 0.07029 -2.28669 0.**

C	**2.86601 -1.15741 0.**	**C**	**2.49407 0.64554 0.**
C	**2.86601 -2.56001 0.**	**C**	**3.74519 0.15266 0.**
C	**4.80004 2.9528 0.**	**C**	**-2.47562 0.52426 0.**
H	**3.52805 1.10093 0.**	**H**	**-0.05056 1.58311 0.**
H	**5.2354 -2.09594 0.**	**H**	**2.20078 -2.09188 0.**
H	**7.33571 1.49914 0.**	**H**	**-2.08855 -2.19732 0.**
H	**7.33039 -1.15586 0.**	**H**	**0.1077 -3.37261 0.**
H	**2.00088 -2.56001 0.**	**H**	**3.07191 2.48537 0.**
H	**2.866 -3.47094 0.**	**H**	**4.61018 0.8108 0.**
H	**3.69912 -2.56002 0.**	**H**	**3.94557 -0.91058 0.**
H	**4.08794 4.45095 0.**	**Li**	**-5.07826 0.85778 0.**

Optimized Cartesian Coordinates (Å)

B3LYP/6-311G(d,p),

3ABA-Ni **X Y Z** **3ABA-Ni/ SCF: -735.210141217 a.u**	3ABA-K **X Y Z** 3ABA - K **SCF -1172.81809724 a.u**
O 2.23524 1.99509 0.	**O 2.23524 1.99509 0.**
O -3.5716 -0.28331 0.	**O -3.5716 -0.28331 0.**
O -2.57525 1.73627 0.	**O -2.57525 1.73627 0.**
C 1.24117 -0.14901 0.	**C 1.24117 -0.14901 0.**
C 0. 0.50158 0.	**C 0. 0.50158 0.**

C	**-1.19454**	**-0.23222**	**C**	**-1.19454**	**-0.23222**
C	**1.25682**	**-1.55643**	**C**	**1.25682**	**-1.55643**
C	**-1.16325**	**-1.63248**	**C**	**-1.16325**	**-1.63248**
C	**0.07029**	**-2.28669**	**C**	**0.07029**	**-2.28669**
C	**2.49407**	**0.64554**	**C**	**2.49407**	**0.64554**
C	**3.74519**	**0.15266**	**C**	**3.74519**	**0.15266**
C	**-2.47562**	**0.52426**	**C**	**-2.47562**	**0.52426**
H	**-0.05056**	**1.58311**	**H**	**-0.05056**	**1.58311**
H	**2.20078**	**-2.09188**	**H**	**2.20078**	**-2.09188**
H	**-2.08855**	**-2.19732**	**H**	**-2.08855**	**-2.19732**
H	**0.1077**	**-3.37261**	**H**	**0.1077**	**-3.37261**
H	**3.07191**	**2.48537**	**H**	**3.07191**	**2.48537**
H	**4.61018**	**0.8108**	**H**	**4.61018**	**0.8108**
H	**3.94557**	**-0.91058**	**H**	**3.94557**	**-0.91058**
Na	**-5.21378**	**0.96042**	**K**	**-5.716**	**1.34078**