TABLE 1S: Starting geometric parameters for geometry optimization of the $P2_1/n$ model. Cell parameters: A=4.17000000Å, B=7.39000000Å, C=2.46000000Å, α=90.000000, β=90.600000, γ=90.000000

	X/A	Y/B	Z/C
C	6.290000000000E-02	2.830000000000E-02	2.407000000000E-01
C	4.371000000000E-01	-4.717000000000E-01	-2.407000000000E-01
C	-6.290000000000E-02	-2.830000000000E-02	-2.407000000000E-01
C	-4.371000000000E-01	4.717000000000E-01	2.407000000000E-01
H	2.706000000000E-01	1.217000000000E-01	2.407000000000E-01
H	2.294000000000E-01	-3.783000000000E-01	-2.407000000000E-01
H	-2.706000000000E-01	-1.217000000000E-01	-2.407000000000E-01
H	-2.294000000000E-01	3.783000000000E-01	2.407000000000E-01

TABLE 2S: Starting geometric parameters for geometry optimization of the $P2_1/a$ model. Cell parameters: A=4.17000000Å, B=7.39000000Å, C=2.46000000Å, α=90.000000, β=90.600000, γ=90.000000

	X/A	Y/B	Z/C
C	6.290000000000E-02	2.830000000000E-02	2.407000000000E-01
C	4.371000000000E-01	-4.717000000000E-01	2.593000000000E-01
C	-6.290000000000E-02	-2.830000000000E-02	-2.407000000000E-01
C	-4.371000000000E-01	4.717000000000E-01	-2.593000000000E-01
H	2.706000000000E-01	1.217000000000E-01	2.407000000000E-01
H	2.294000000000E-01	-3.783000000000E-01	2.593000000000E-01
H	-2.706000000000E-01	-1.217000000000E-01	-2.407000000000E-01
H	-2.294000000000E-01	3.783000000000E-01	-2.593000000000E-01