Supplementary Material

UV Irradiation and Near Infrared Characterization of Laboratory Mars Soil Analog Samples: the case of Phthalic Acid, Adenosine 5'-Monophosphate, L-Glutamic Acid and L-Phenylalanine Adsorbed onto the Clay Mineral Montmorillonite in the presence of Magnesium Perchlorate

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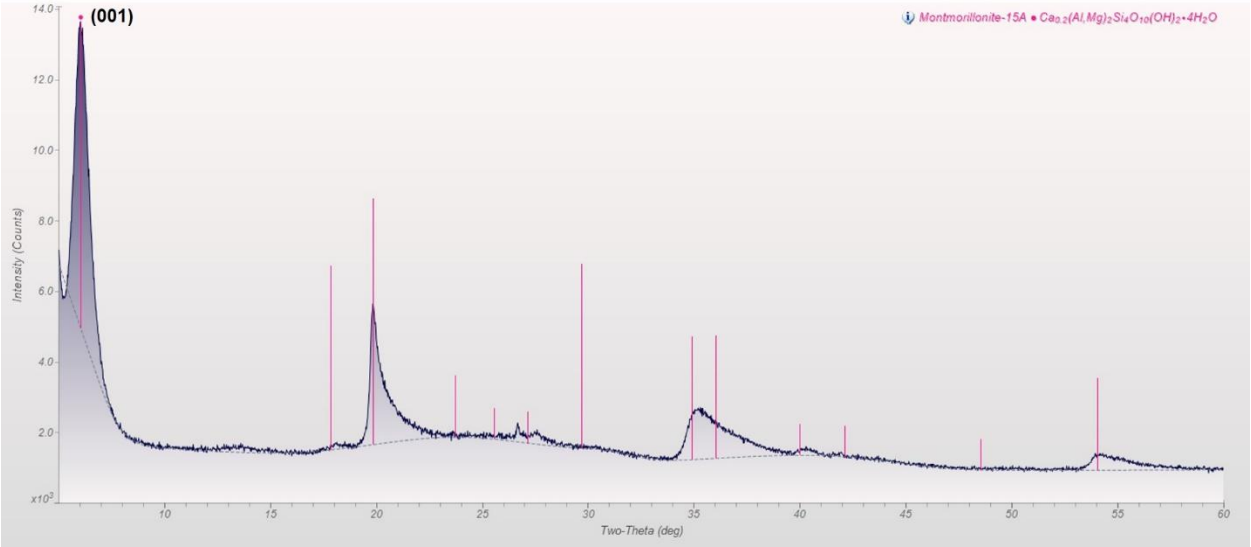
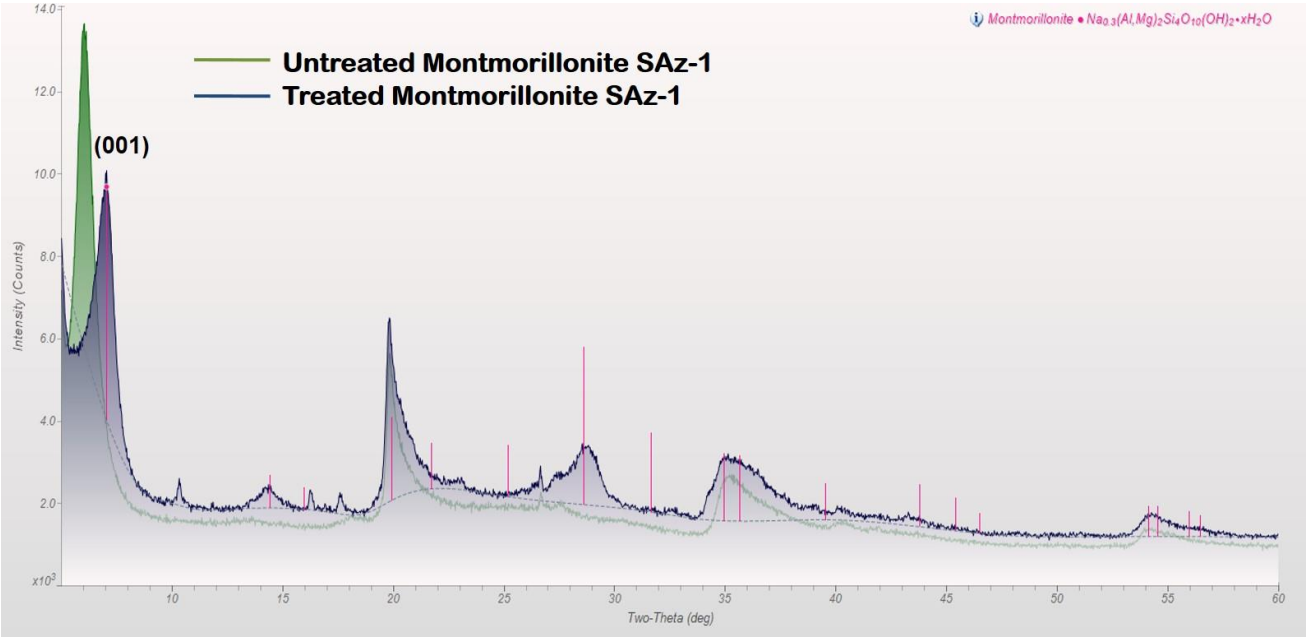
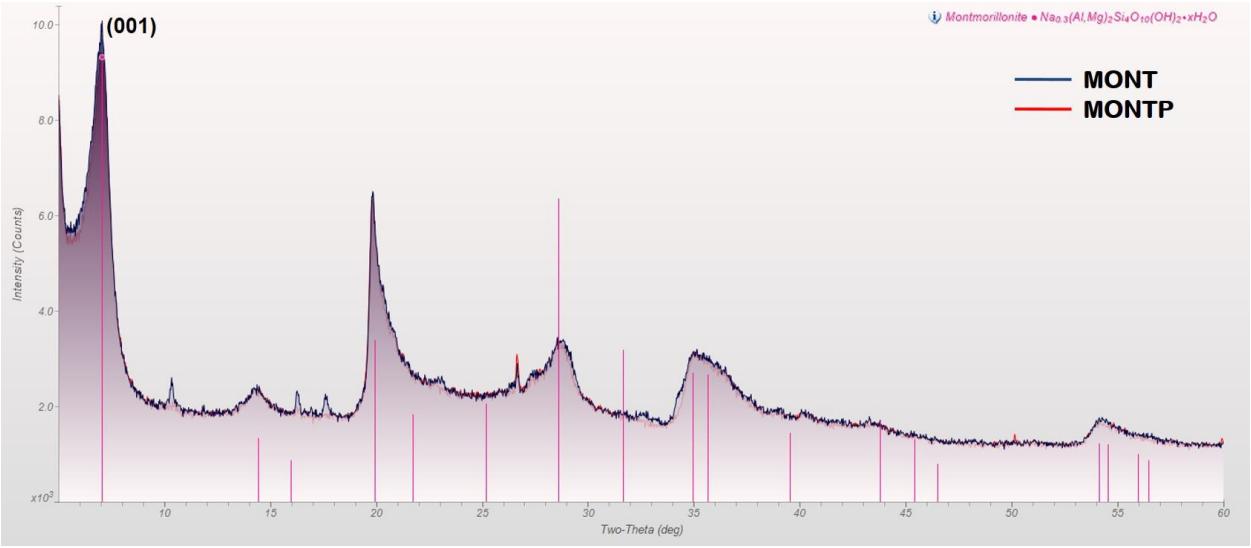


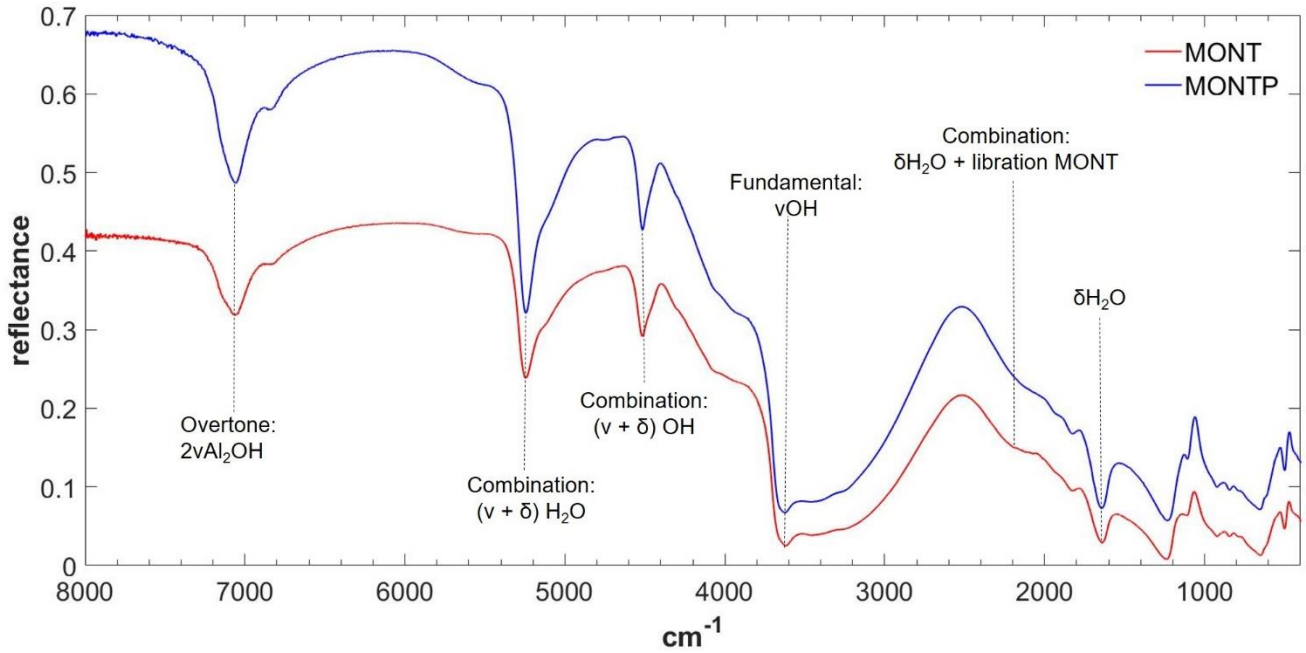
Supplementary Figure 1. XRD pattern of untreated montmorillonite.



Supplementary Figure 2. XRD pattern of untreated montmorillonite, compared with XRD pattern of montmorillonite treated to remove organic contamination.

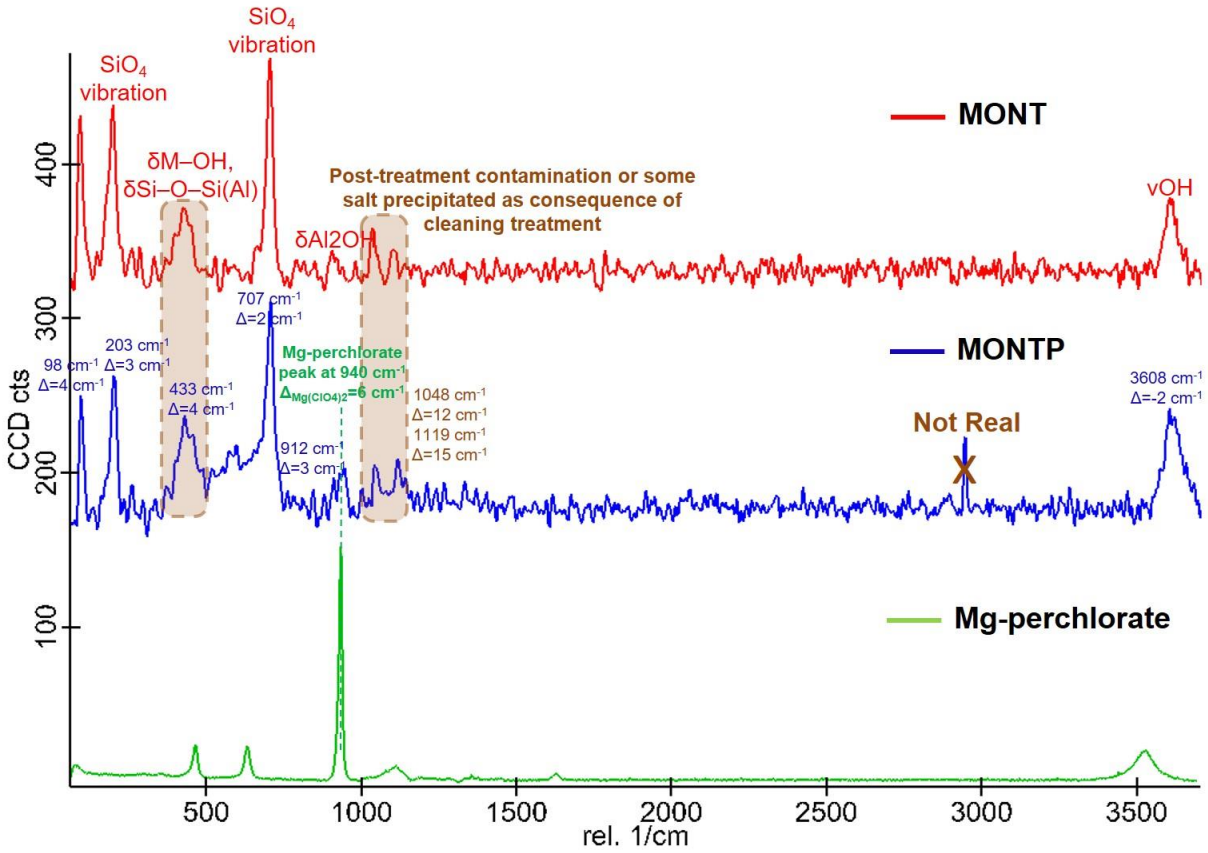


Supplementary Figure 3. XRD patterns of montmorillonite (MONT) and montmorillonite doped with 1 wt% magnesium perchlorate (MONTP).

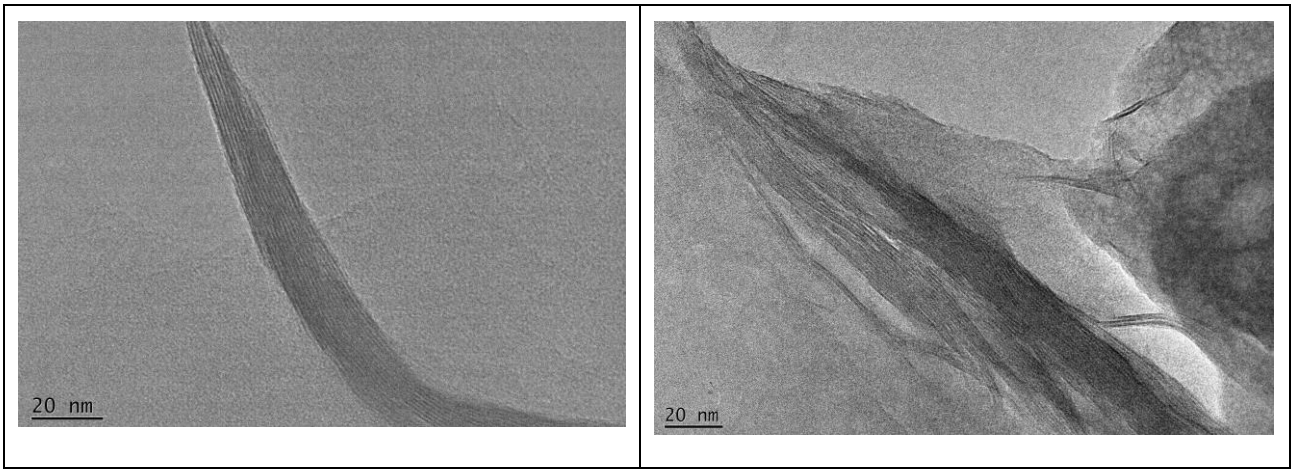


Supplementary Figure 4. IR characterization of montmorillonite (MONT) and montmorillonite

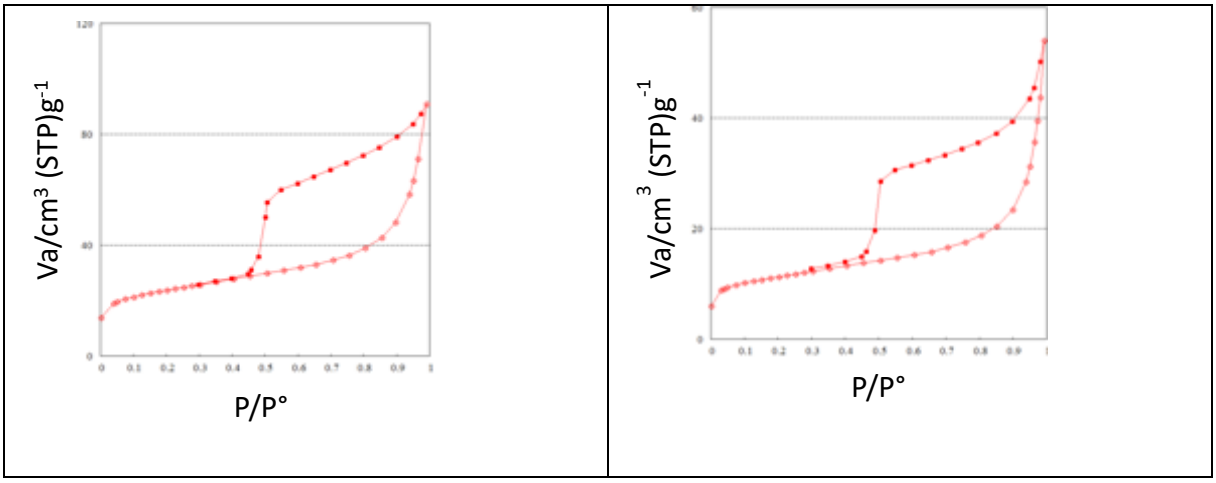
doped with 1 wt% magnesium perchlorate (MONTP). Assignments are based on Refs. (BISHOP et al., 2002; Madejová et al., 2006; Madejová, 2003).



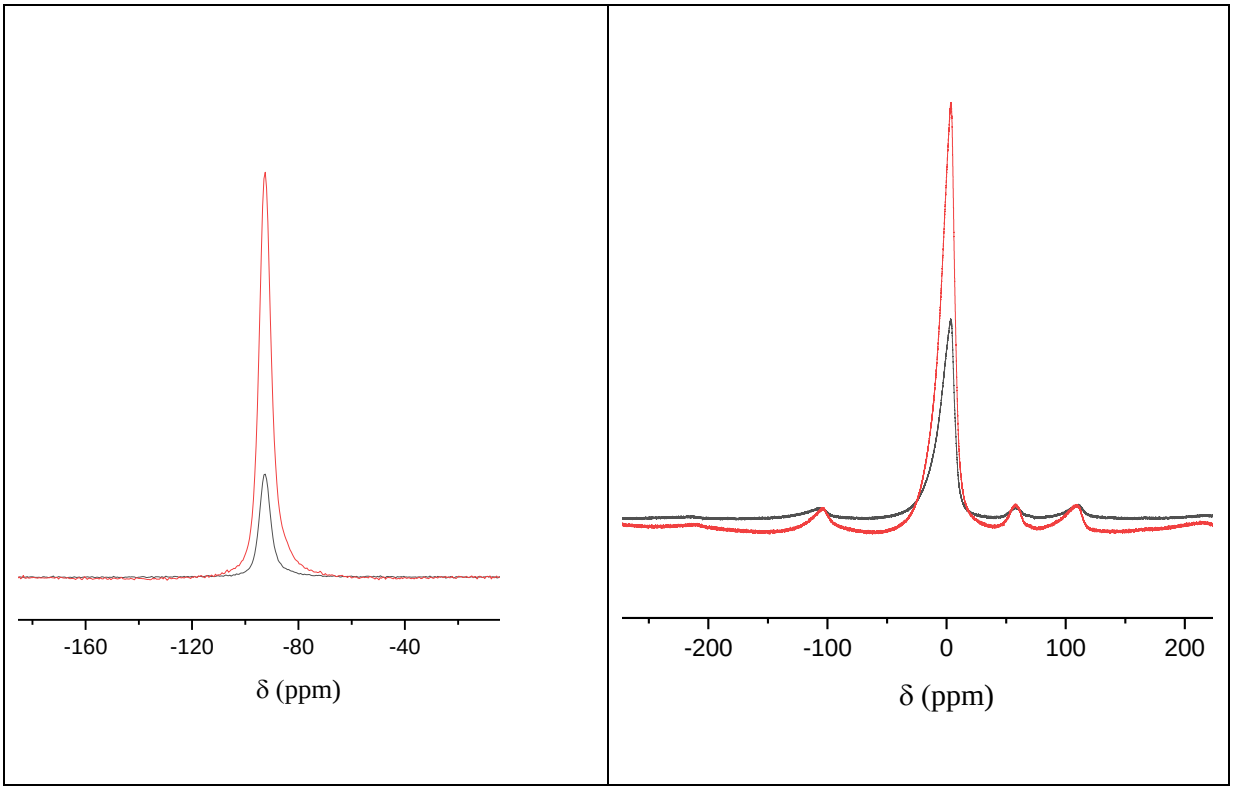
Supplementary Figure 5. Raman characterization of montmorillonite (MONT) and montmorillonite doped with 1 wt% magnesium perchlorate (MONTP).



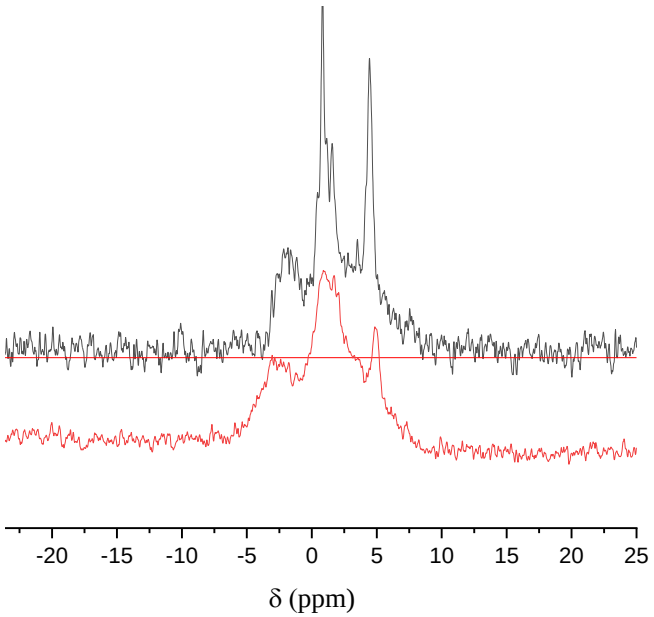
Supplementary Figure 6. TEM micrograph of montmorillonite doped with 1 wt% magnesium perchlorate (MONTP) on the right, and montmorillonite (MONT) on the left.



Supplementary Figure 7. N2 adsorption-desorption isotherms for montmorillonite doped with 1 wt% magnesium perchlorate (MONTP) on the right, and montmorillonite (MONT) on the left.



Supplementary Figure 8. On the right, NMR spectra of ^{27}Al MAS NMR of MONT (red) and MONTP (black); on the left, ^{29}Si HP-DEC of MONT (red) and MONTP (black).



Supplementary Figure 9. ^{1}H-NMR spectra of MONT (red) and MONTP (black).

Supplementary Table 1. Tentative assignment of experimental NIR bands of pure molecules in the solid state based on comparison with vibrational wavenumbers and intensities calculated at anharmonic level using GVPT2 method and B3LYP-D3/SNSD level of theory. Band position is taken from maximum of the peak, obtained by convolution of all single fundamental and non-fundamental transitions with the Lorenzian function of the half-width at half maxima of 10 cm^{-1}, and intensity is calculated as sum of all contributions in the peak zone.

Mode (n)	E (harm)	E (anharm)	I (harm)	I (anharm)	Band position	Band intensity	Assignment	ῡ	I
AMP GVPT2 B3LYP-D3/SNSD								AMP solid state exp.	
7(2)	6508	6097		0.3			Overtone: 2νC_8H	6150	m
48(1)+1(1)	4893	4629		2.5	4629	3.5	Combination: $\nu OH_{phosp}+\delta OH_{phosp}$	4640	ms
42(1)+4(1)	4792	4521		1.5	4522	4.0	Combination: $\nu OH_{phosp}+\delta OH_{phosp}$		
53(1)+2(1)	4746	4524		1.7			Combination: $\nu_{asym}NH_2+\delta C_8H,\delta_{rock}NH_2$		
10(1)	3089	2957	6.9	16.8	2956	30.8	Fundamental: $\nu_{asym}CH$	2945	m
11(1)	3052	2935	23.7	8.6	2934	12.1	Fundamental: $\nu_{sym}CH_2$	2916	mw
12(1)	3036	2907	26.7	47.1			Fundamental: νCH	2895	w
13(1)	3020	2891	37.6	12.0	2887	66.9	Fundamental: $\nu_{sym}CH$	2883	w
GLU GVPT2 B3LYP-D3/SNSD								GLU solid state exp.	

2(2)	7154	6711		0.8			Overtone: $2\nu_{asym}NH_2$	6708	m
12(1)+2(1)	5235	4962		2.0			Combination: $\delta_{sciss}NH_2+\nu_{asym}NH_2$	5100	vs
5(1)	3124	2992	10.0	9.4	2978	22.11	Fundamental: $\nu_{asym}CH_2$	2972	m
6(1)	3107	2972	4.1	6.4			Fundamental: $\nu_{asym}CH_2$		
7(1)	3068	2939	9.5	7.9			Fundamental: $\nu_{sym}CH_2$		
8(1)	3052	2926	9.5	12.2	2930	26.4	Fundamental: $\nu_{sym}CH_2$, CH	2937	mw
9(1)	3036	2911	9.8	2.6			Fundamental: $\nu_{sym}CH_2$,CH		
14(2)	2962	2865		2.4	2863.00	5.7	Overtone: $2\delta_{sciss}CH_2$	2860	mw
14(1)+13(1)	2971	2860		3.3			Combination: $\delta_{sciss}CH_2+\delta_{sciss}CH_2$		
PHE GVPT2 B3LYP-D3/SNSD								PHE solid state exp.	
4(2)	6389	6003		1.3			Overtone: $2\nu CH_{aromatic}$	5960	vs
14(1)+5(1)	4834	4681		0.1	4693	0.40	Combination: ν ring+$\nu CH_{aromatic}$	4671	s
15(1)+5(1)	4811	4644		0.1	4639	0.9	Combination: ν ring+$\nu CH_{aromatic}$	4637	vs c
15(1)+8(1)	4785	4616		0.4	4616	0.4	Combination: ν ring+$\nu CH_{aromatic}$	4581	s
35(1)+6(1)	4191	4048		0.7	4045	44.0	Combination: ring def + $\nu CH_{aromatic}$	4045	s
6(1)	3175	3080	6.8	0.5	3090	31.64	Fundamental: $\nu CH_{aromatic}$	3120	s b
7(1)	3165	3054	0.9	13.9			Fundamental: $\nu CH_{aromatic}$	3049	vvw wb
5(1)	3183	3039	24.8	17.2			Fundamental: $\nu CH_{aromatic}$	3011	vvw wb
9(1)	3098	2963	12.7	11.2	2969	30.5	Fundamental: $\nu_{asym}CH_2$	2970	m wb
10(1)	3078	2944	6.9	19.2			Fundamental: νCH		
11(1)	3042	2860	15.3	7.4			Fundamental: $\nu_{sym}CH_2$	2874	w wb
19(2)	2833	2758		0.3	2756	1.15	Overtone: δ CH	2748	m wb
PHA GVPT2 B3LYP-D3/SNSD								PHA solid state exp.	
6(2)	6359	5993		1.5		2.35	Overtone: νCH	6158	m
4(2)	6414	6070		0.1	6070	1.6	Overtone: νCH	6050	vs
9(1)+6(1)	4821	4636		0.3	4645	0.8	Combination: ν ring + $\nu CH_{aromatic}$	4679	vs
11(1)+3(1)	4737	4566		0.04			Combination: $\delta CH_{aromatic}+\nu CH_{aromatic}$	4585	ms
18(1)+6(1)	4389	4205		0.2	4190	0.4	Combination: $\delta OH+\nu CH_{aromatic}$	4222	m
35(1)+2(1)	4353	4144		0.4	4130	4.084	Combination: δOH+νOH	4156	vs
41(1)+2(1)	4096	3905		0.06	3902	0.14	Combination: τ molecule + νOH	3910	s
5(1)	3194	3063	7.3	9.4	3060	19.5	Fundamental: νCH	3088	s
14(1)+9(1)	3008	2934		0.5	2933	1.2	Combination: δOH + ν ring	2905	m
13(1)+1(1)	2897	2820		0.2	2820	0.6	Combination: δOH + νOH	2814	m

Legend: ϋ = wavenumber in cm^{-1}; E = Energy; harm = harmonic; anharm = anharmonic; I = Intensity of the band; phosp = phosphate group; ν = stretching vibrational mode; δ = bending vibrational mode; τ = torsional vibrational mode; def = deformation vibrational mode; sciss = scissoring in-plane vibrational mode; wagg = wagging out-of-plane vibrational mode; s = strong band; m = medium band; w = weak band; vw = very weak band; vvw = extremely weak band; c = convolution of peaks; b = broad band; wb = within broad band.