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Supporting Information

Raman spectroscopy-in situ characterization of reversibly intercalated oxygen vacancies in α -MoO₃

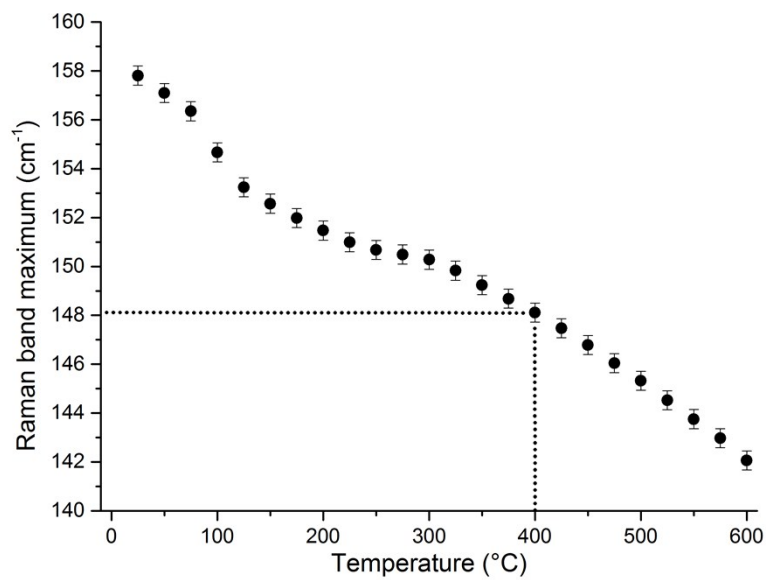
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19 Table S1. Indexation of the diffraction peaks of the MoO₃ sample observed at 22 °C under
 20 20 % O₂/He, according to ICDD files 5-0508 (α -MoO₃) and 47-1320 (β -MoO₃).

2θ (°)	d_{hkl} (Å)	Indexing
12.824	6.94	(020) α -MoO ₃
23.460	3.81	(110) α -MoO ₃
25.818	3.47	(040) α -MoO ₃
27.432	3.268	(021) α -MoO ₃
29.526	3.041	(130) α -MoO ₃
33.278	2.706	(101) α -MoO ₃
33.834	2.663	(111) α -MoO ₃
35.636	2.532	(041) α -MoO ₃
39.152	2.313	(060) α -MoO ₃
39.944	2.269	(150) α -MoO ₃
45.986	1.984	(200) α -MoO ₃
46.536	1.962	(210) α -MoO ₃
48.470	1.888	(2 0 -2) β-MoO₃
49.470	1.852	(002) α -MoO ₃
51.332	1.789	(021) β-MoO₃
52.278	1.759	(161) α -MoO ₃
52.638	1.748	(201) β-MoO₃
53.070	1.735	(211) α -MoO ₃
54.018	1.706	(221) α -MoO ₃
55.446	1.666	(112) α -MoO ₃
56.630	1.634	(042) α -MoO ₃
57.906	1.601	(171) α -MoO ₃
59.124	1.571	(081) α -MoO ₃
64.830	1.446	(062) α -MoO ₃
65.210	1.438	(190) α -MoO ₃
67.908	1.387	(0 10 0) α -MoO ₃
69.860	1.353	(202) α -MoO ₃



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23 Figure S1. T_b Raman band frequency as a function of temperature for α - MoO_3 under O_2 .

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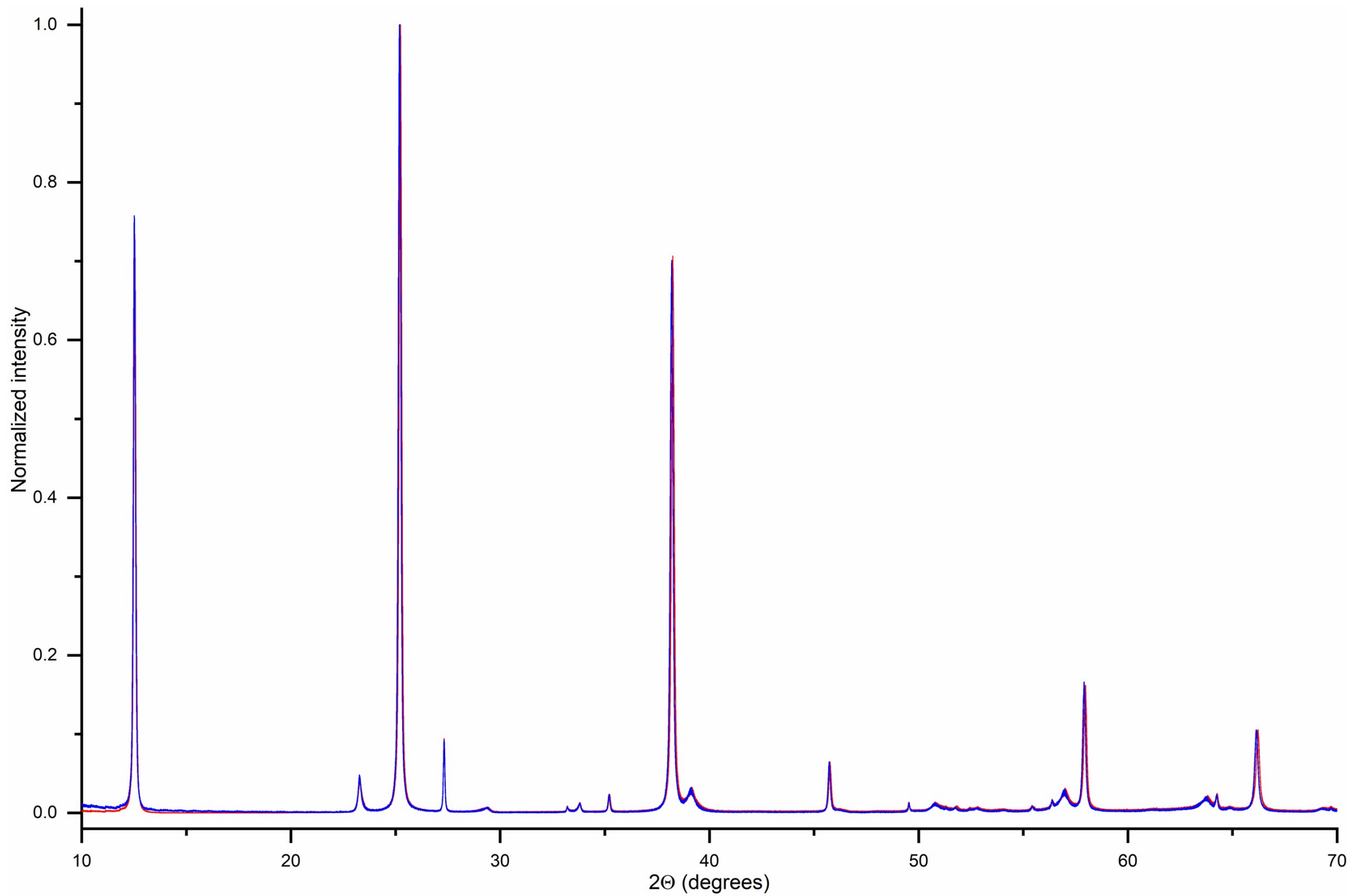
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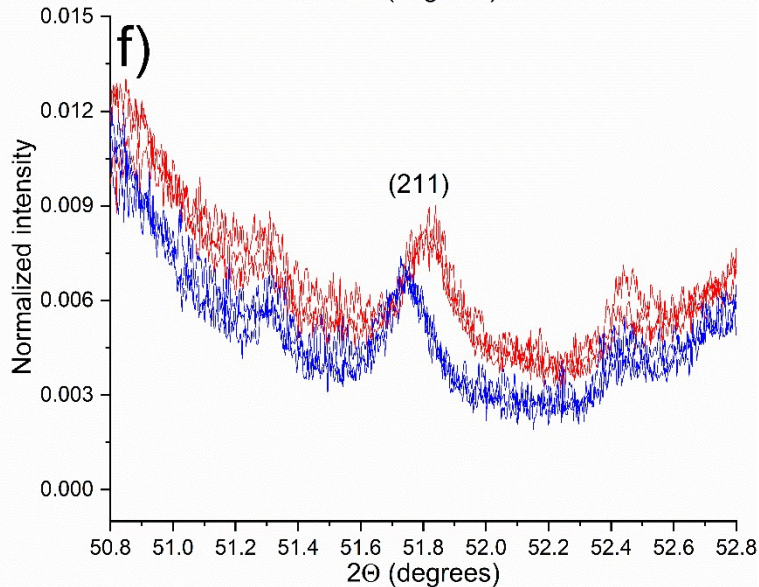
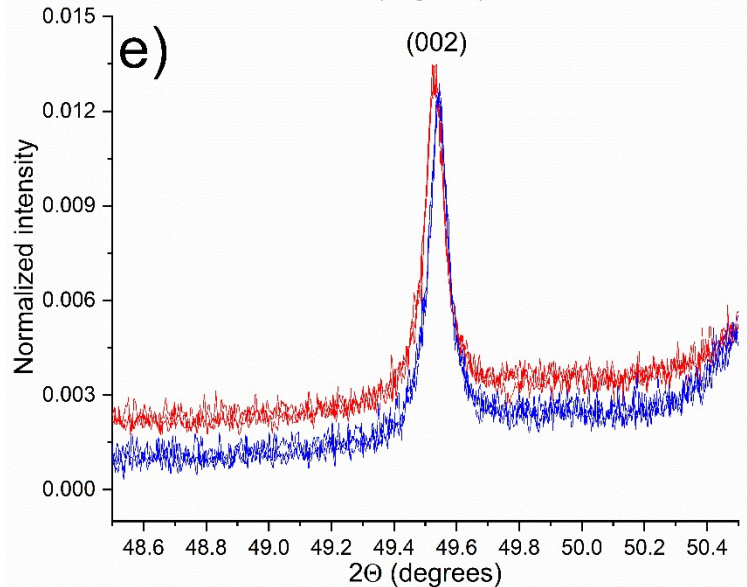
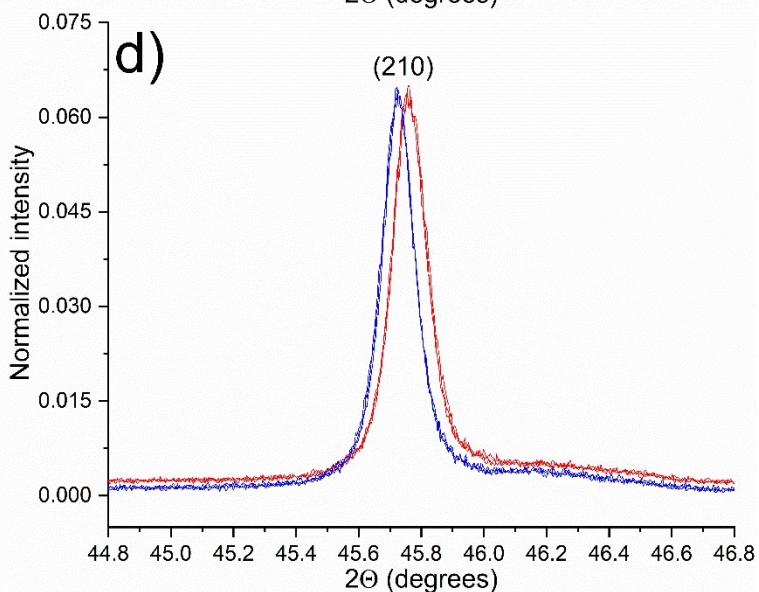
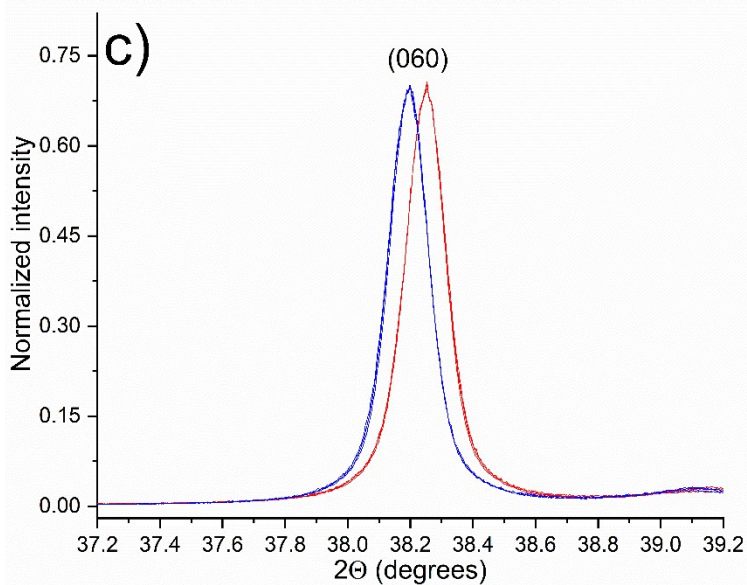
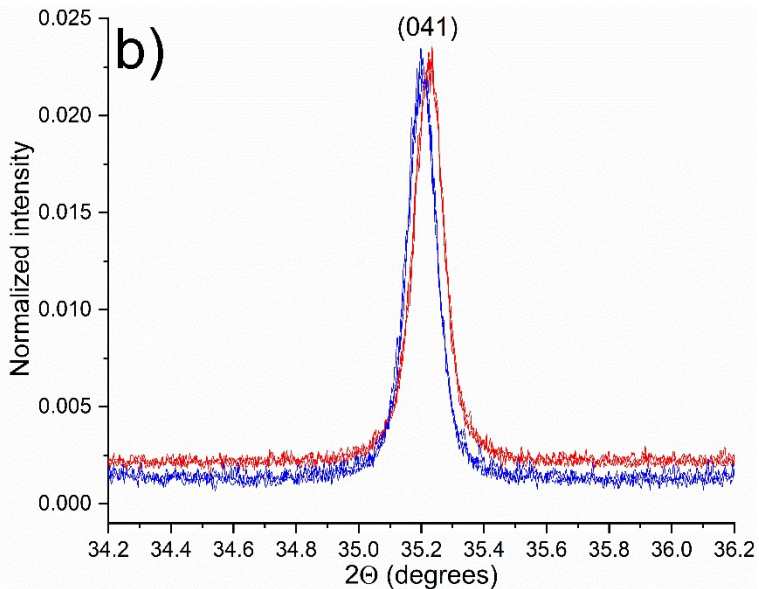
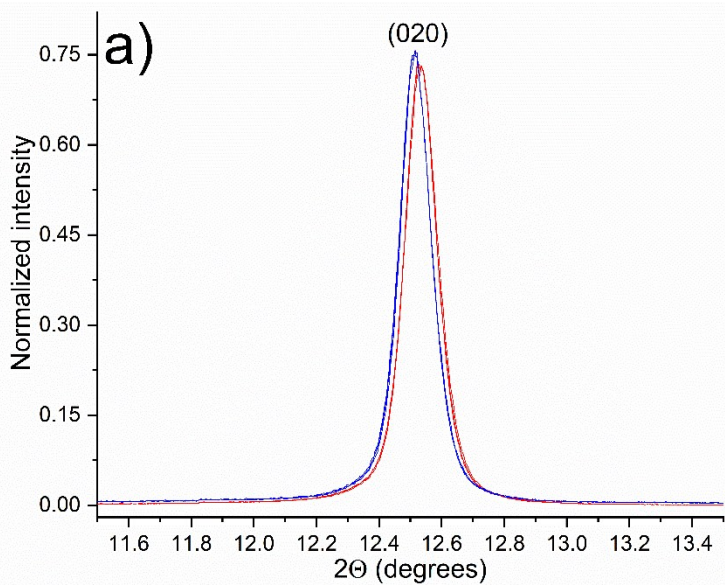
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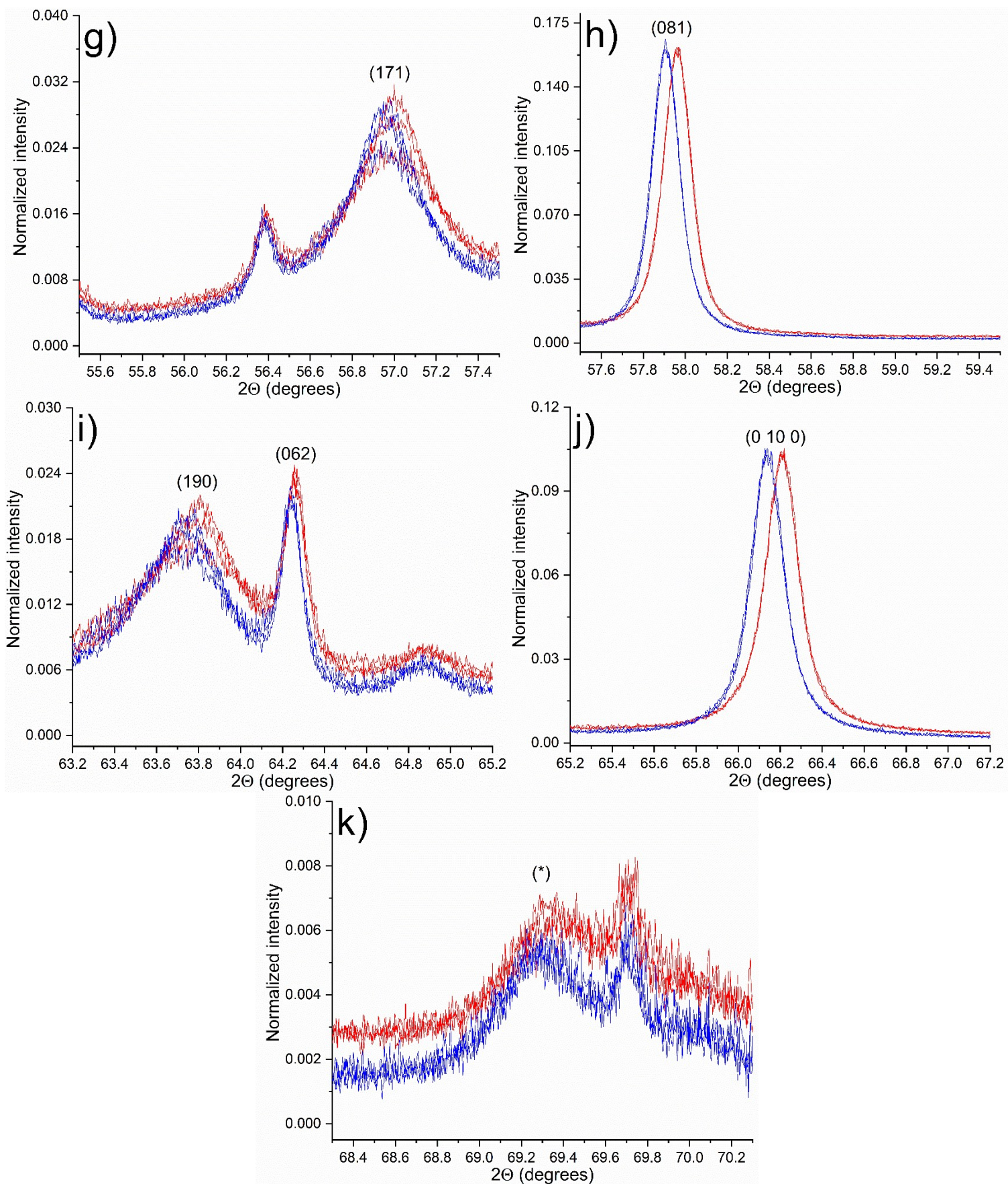
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3 Figure S2. Diffractograms of MoO_3 sample obtained at 400°C . The blue ones were obtained after O_2 exposure, and the red ones were obtained after H_2 exposure.





0 Figure S3. Amplification of diffractograms in Figure S2 to show peaks displacements. The blue ones were obtained
 1 after O_2 exposure, and the red ones were obtained after H_2 exposure. The last peak could not be indexed (k).