

Explosive versus Thermite Behavior in Iron(0) Aerogels Infiltrated with Perchlorates

Nicholas Leventis^{*,1}, Suraj Donthula¹, Chandana Mandal¹, Michael S. Ding^{*,2} and
Chariklia Sotiriou-Leventis^{*,1}

1. Department of Chemistry, Missouri University of Science and Technology, Rolla, MO 65409, U.S.A. leventis@mst.edu; cslevent@mst.edu
2. Electrochemistry Branch, Army Research Laboratory, 2800 Powder Mill Road, Adelphi, MD 20783, U.S.A. michael.s.ding.civ@mail.mil

Supporting Information

Table S.1. Cumulative XRD analysis and thermochemical data of perchlorate-loaded samples before and after ignition under various conditions

Ignition Movies

Fe-temp loaded with LiClO₄

Ignition in open air

Movie S.AIR.1...Fe-350-LiClO₄
Movie S.AIR.2...Fe-400-LiClO₄
Movie S.AIR.3...Fe-600-LiClO₄
Movie S.AIR.4...Fe-800-LiClO₄
Movie S.AIR.5...Fe-950-LiClO₄
Movie S.AIR.6...Fe-1100-LiClO₄
Movie S.AIR.7...Fe-1200-LiClO₄
Movie S.AIR.8...Fe-1300-LiClO₄

Ignition in sealed tubes under vacuum

Movie S.VAC.1...Fe-400-LiClO₄
Movie S.VAC.2...Fe-600-LiClO₄
Movie S.VAC.3...Fe-700-LiClO₄
Movie S.VAC.4...Fe-800-LiClO₄
Movie S.VAC.5...Fe-950-LiClO₄

Ignition in sealed tubes under N₂

Movie S.N2.1...Fe-350-LiClO₄
Movie S.N2.2...Fe-700-LiClO₄
Movie S.N2.3...Fe-800-LiClO₄

Fe-temp loaded with NaClO₄

Movie S.Na.1...Fe-400-NaClO₄
Movie S.Na.2...Fe-600-NaClO₄
Movie S.Na.3...Fe-1000-NaClO₄

Fe-temp loaded with KClO₄

Movie S.K.1...Fe-400-KClO₄
Movie S.K.2...Fe-600-KClO₄
Movie S.K.3...Fe-1000-LClO₄

Table S.1. Cumulative XRD analysis and TGA data of perchlorate-loaded samples before and after ignition under various conditions

Sample ^a	Fe(0) perchlorate (mol/mol) ^b	$\frac{\text{Fe}_{\text{reacted}}}{\text{Fe}_{\text{initial}}}$ (mol/mol) ^c	Fe (mol%) ^d	FeO (mol%) ^d	Fe ₃ O ₄ (mol%) ^d	Fe ₂ O ₃ (mol%) ^d	ΔH (kcal/mol) ^e theoretical [experimental]
Loaded with LiClO ₄							
Fe-300 ^f	-	-	-	-	-	-	-
Fe-350	2.675	1.000	0	0	100	0	-91.298
Fe-400	2.929	1.000	0	100	0	0	-66.639
Fe-500	2.959	1.000	0	0	42	58	-95.953
Fe-600	2.634	0.922	11	68	21	0	-78.527
Fe-600-BC	2.634	0.898	11	83	0	6	-71.066 [-60.1]
Fe-700	2.640	^g	^g	^g	^g	^g	-66.639
Fe-700-BC	2.640	0.887	11	89	0	0	-66.639 [-58.3]
Fe-700-vac	2.640	0.899	10	90	0	0	-66.639
Fe-800	1.777	0.537	67	0	11	22	-96.675
Fe-800-BC	1.777	0.898	11	83	0	6	-71.066 [-57.5]
Fe-800-vac	1.777	0.734	27	73	0	0	-66.639
Fe-900	5.369	1.000	0	0	100	0	-91.298
Fe-950	5.552	1.000	0	0	100	0	-91.298
Fe-950-vac	5.552	0.203	82	15	0	3	-75.537

Fe-1000	4.252	0.332	67	33	0	0	-66.639
Fe-1100	6.436	0.360	64	36	0	0	-66.639
Fe-1200	6.634	0.705	36	52	12	0	-76.594
Fe-1300	12.836	0.946	15	0	85	0	-91.298
Loaded with NaClO₄							
Fe-400	7.137	0.986	3	0	24	73	-97.794
Fe-600	7.472	0.828	32	0	21	47	-97.177
Fe-1000	21.448	0.263	89	0	11	0	-91.322
Loaded with KClO₄							
Fe-400	12.920	0.671	40	50	10	0	-74.403
Fe-600	162.871	0.202	90	0	3	7	-95.126
Fe-1000	314.407	0.220	91	0	9	0	-89.394

^a Samples were ignited in air unless otherwise noted (BC: in a bomb calorimeter; vac: in evacuated sealed ampules).

^b Determined gravimetrically.

^c Calculated from the iron products in the residue after ignition via:

$[100 - \% \text{Fe}_{\text{in-residue}}] / 100 \times [\% \text{Fe}_{\text{in-residue}} + \% \text{FeO} + 2 \times \% \text{Fe}_2\text{O}_3 + 3 \times \% \text{Fe}_3\text{O}_4]$. All % in mol/mol from ^d.

^d Via XRD and quantitative phase analysis.

^e Based on the amount of iron reacted.

Theoretical values were calculated from standard heats of formation assuming no air (O₂) participation and stoichiometrically sufficient amount of perchlorate: (ΔH_f)_{LiCl} = -97.679 kcal/mol, (ΔH_f)_{LiClO₄} = -91.057 kcal/mol, (ΔH_f)_{KCl} = -104.324 kcal/mol, (ΔH_f)_{KClO₄} = -103.439 kcal/mol, (ΔH_f)_{NaCl} = -98.277 kcal/mol, (ΔH_f)_{NaClO₄} = -91.609 kcal/mol, (ΔH_f)_{Fe} = 0 kcal/mol, (ΔH_f)_{FeO} = -65.008 kcal/mol, (ΔH_f)_{Fe₂O₃} = -196.984 kcal/mol, (ΔH_f)_{Fe₃O₄} = -267.298 kcal/mol.

Experimental values were measured with a bomb calorimeter.

^f Sample consisted mostly of oxides.

^g No residue could be recovered.