Reverse Water Gas Shift by Chemical Looping with Iron-Substituted Hexaaluminate Catalysts

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Supplementary information

Table S1. Atomic positions, coordinates and positions occupancies in $BaFeHF_{co\text{-}pre}$ material: $Ba_{0.9}Fe_{11.0}O_{17.4}$ (a=b=5.902Å; c=23.235Å)

Atom	Position	x	y	z	Occupancy
Ba	2d	2/3	1/3	1/4	0.90
Fe_1	2a	0	0	0	0.92
Fe_2	4f	1/3	2/3	0.02878	0.84
Fe_3	4f	1/3	2/3	0.18781	0.90
Fe_4	4e	0	0	0.24583	0.50
Fe_5	12k	0.16861	0.33712	-0.10807	0.93
O_1	6h	-0.08886	-0.16012	1/4	0.85
O_2	12k	0.14881	0.29762	0.05587	1.0
O_3	12k	0.48510	0.97020	0.15057	0.84
O_4	4e	0	0	0.35605	0.96
O_5	4f	1/3	2/3	-0.04904	0.93

Table S2. Atomic positions, coordinates and positions occupancies in $BaFeHF_r$ material: $Ba_{0.8}Fe_{11.0}O_{17.3}$ (a=b=5.801Å; c=23.361Å)

Atom	Position	x	y	z	Occupancy
Ba	2d	2/3	1/3	1/4	0.80
Fe_1	2a	0	0	0	0.86
Fe_2	4f	1/3	2/3	0.03888	0.80
Fe_3	4f	1/3	2/3	0.18493	0.95
Fe_4	4e	0	0	0.21574	0.50
Fe_5	12k	0.15272	0.30744	-0.11567	0.94
O_1	6h	-0.16389	-0.32778	1/4	0 .85
O_2	12k	0.15215	0.30430	0.06190	1.0
O_3	12k	0.49047	0.98094	0.17714	0.84
O_4	4e	0	0	0.38418	0.96
O_5	4f	1/3	2/3	-0.08814	0 .93