Manuscript-ID-2011-00662m; Supporting information:

Investigation of counter ion influence on an octahedral IrH_6-complex in the solid state hydrides $AAeIrH_6$ (A = Na, K and Ae = Ca, Sr, Ba and Eu) with a new structure type.

K. Kadir*, D. Moser, M. Münzel and D. Noréus

Department of Materials and Environmental Chemistry, Arrhenius Laboratory, Stockholm University, S-106 91 Stockholm, Sweden

*E-mail:karim@ mmk.su.se
Tel:- (46) 8 16 23 83
Fax:- (46) 8 16 31 18

Table: 1.
Observed, calculated,$1/d^2$-values and intensities for $NaCaIrH_6$ by using Guinier-Hägg x-ray diffraction Cu $K\alpha_1$ radiation and with Si as the internal standard at 293K.

h	*k*	*l*	$1/d^2_{obs}$.	$1/d^2_{cal}$.	I_{obs}.
1	1	1	.056821	.057001	100
2	0	0	.075854	.076006	18
2	2	0	.151710	.152005	82
3	1	1	.208649	.209007	58
2	2	2	.227763	.228014	5
4	0	0	.303739	.304010	14
3	3	1	.360619	.361017	22
4	2	0	.379823	.380019	10
4	2	2	.455820	.456016	32
5	1	1	.512986	.513026	22
4	4	0	.608595	.608030	11
5	3	1	.665647	.665029	25
6	0	0	.683922	.684037	4
5	3	3	.817733	.817042	9

Table: 2.
Observed, calculated, $1/d^2$-values and intensities for $NaSrIrH_6$ by using Guinier-Hägg x-ray diffraction Cu $K\alpha_1$ radiation and with Si as the internal standard at 293.

h	*k*	*l*	$1/d^2_{obs.}$	$1/d^2_{cal.}$	$I_{obs.}$
1	1	1	.053415	.053503	92
2	0	0	.071275	.071334	4
2	2	0	.142545	.142668	100
3	1	1	.196011	.196172	55
4	0	0	.285277	.285343	18
3	3	1	.338628	.338840	23
4	2	0	.356370	.356670	3
4	2	2	.427816	.428008	41
5	1	1	.481332	.481518	20
4	4	0	.570847	.570680	13
5	3	1	.624377	.624178	23
6	2	0	.714005	.713351	19

Table: 3.
Observed, calculated, $1/d^2$-values and intensities for $NaBaIrH_6$ by using Guinier-Hägg x-ray diffraction Cu $K\alpha_1$ radiation and with Si as the internal standard at 293.
M (13) = 76

h	*k*	*l*	$1/d^2_{obs.}$	$1/d^2_{cal.}$	$I_{obs.}$
1	1	1	.049172	.049271	86
2	0	0	.065564	.065552	2
2	2	0	.131131	.131036	100
3	1	1	.180304	.180240	53
4	0	0	.262258	.262120	21
3	3	1	.311431	.311351	23
4	2	2	.393389	.393252	40
5	1	1	.442555	.442439	18
4	4	0	.524512	.524417	12
5	3	1	.573689	.573689	17
6	2	0	.655638	.655724	18
5	3	3	.704812	.705146	6
4	4	4	.786768	.786870	3

Table: 4.
Observed, calculated, $1/d^2$-values and intensities for $NaEuIrH_6$ by using Guinier-Hägg x-ray diffraction Cu $K\alpha_1$ radiation and with Si as the internal standard at 293.

h	*k*	*l*	$1/d^2_{obs.}$	$1/d^2_{cal.}$	$I_{obs.}$
1	1	1	.052911	.052855	90
2	0	0	.070378	.070472	8
2	2	0	.140880	.140945	100
3	1	1	.193679	.193801	44
4	0	0	.281997	.281888	20
3	3	1	.334325	.334735	20
4	2	0	.352355	.352355	3
4	2	2	.422335	.422833	35
5	1	1	.475444	.475682	7
4	4	0	.564161	.563772	4
5	3	1	.617184	.616631	17
6	2	0	.704203	.704711	12
5	3	3	.758146	.757575	4

Table: 5.
Observed, calculated, $1/d^2$-values and intensities for $KBaIrH_6$ by using Guinier-Hägg x-ray diffraction Cu $K\alpha_1$ radiation and with Si as the internal standard at 293.
M (13) = 52

h	*k*	*l*	$1/d^2_{obs.}$	$1/d^2_{cal.}$	$I_{obs.}$
1	1	1	.046173	.046178	68
2	0	0	.061624	.061569	2
2	2	0	.123138	.123138	100
3	1	1	.169327	.169319	37
4	0	0	.246247	.246279	20
3	3	1	.292426	.292460	14
4	2	2	.369318	.369428	44
5	1	1	.415598	.415598	12
4	4	0	.492558	.492558	13
5	3	1	.538823	.538741	12
6	2	0	.616008	.615710	20
5	3	3	.662327	.661882	4
4	4	4	.738198	.738840	2

Table: 6.
Observed, calculated, $1/d^2$-values and intensities for $KSrIrH_6$ by using Guinier-Hägg x-ray diffraction Cu $K\alpha_1$ radiation and with Si as the internal standard at 293.

h	k	l	$1/d^2_{obs.}$	$1/d^2_{cal.}$	$I_{obs.}$
1	1	1	.049083	.049152	83
2	0	0	.065512	.065535	4
2	1	1	.098345	.098297	3
2	2	0	.130934	.131068	100
3	1	1	.180149	.180222	67
3	2	1	.229626	.229364	1
4	0	0	.262077	.262131	40
3	3	1	.311317	.311282	32
4	2	0	.327361	.327664	2
4	2	2	.393165	.393202	61
5	1	1	.442296	.442348	26
4	4	0	.524376	.524267	23
5	3	1	.573466	.573424	24
6	2	0	.655552	.655337	30
5	3	3	.704319	.704493	8
4	4	4	.786503	.786401	9

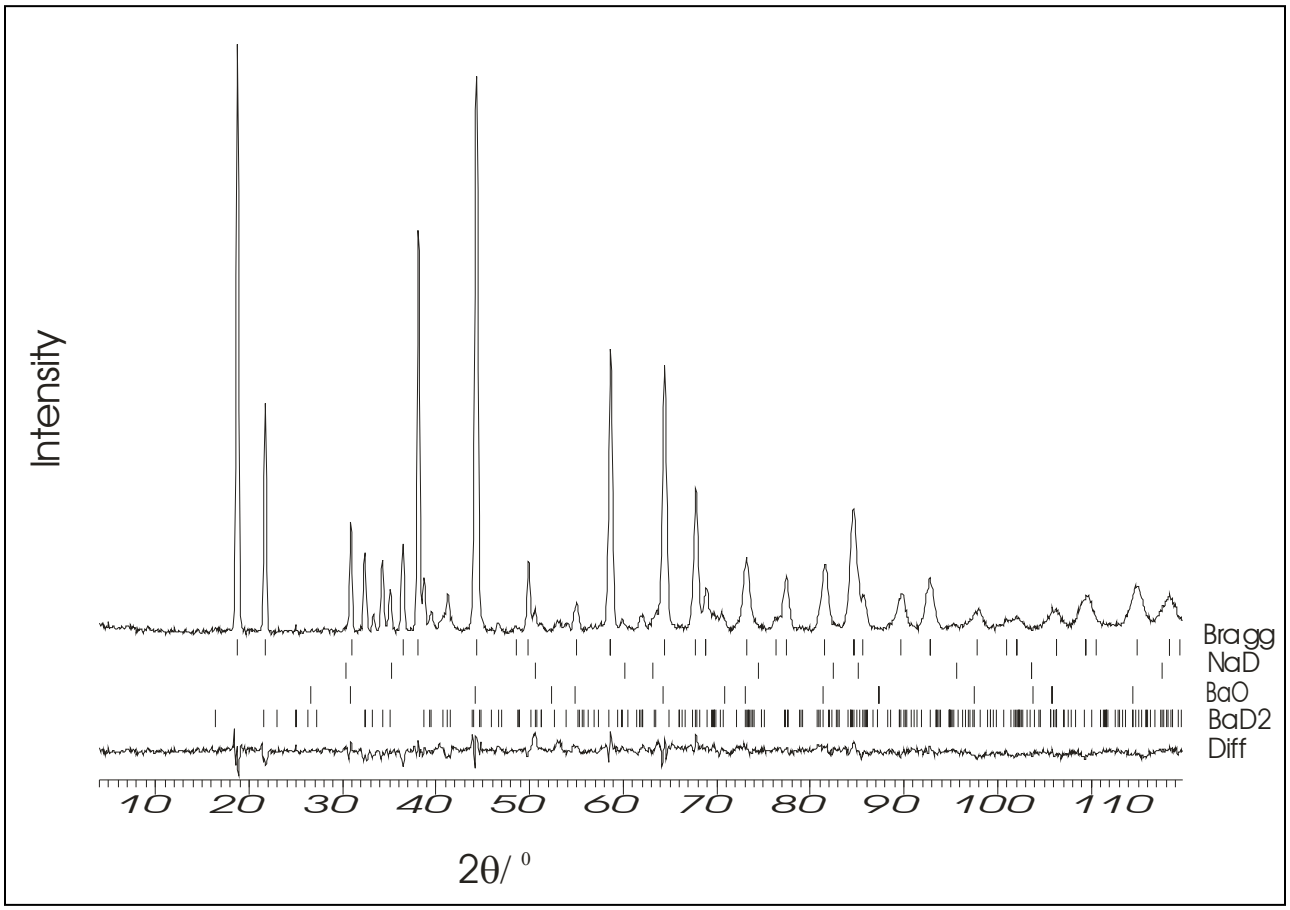

Figure 1.
The difference plot obtained in the profile refinement of the NPD data on $NaBaIrD_6$. BaD_2, NaD and BaO are indicated as an impurity phases.

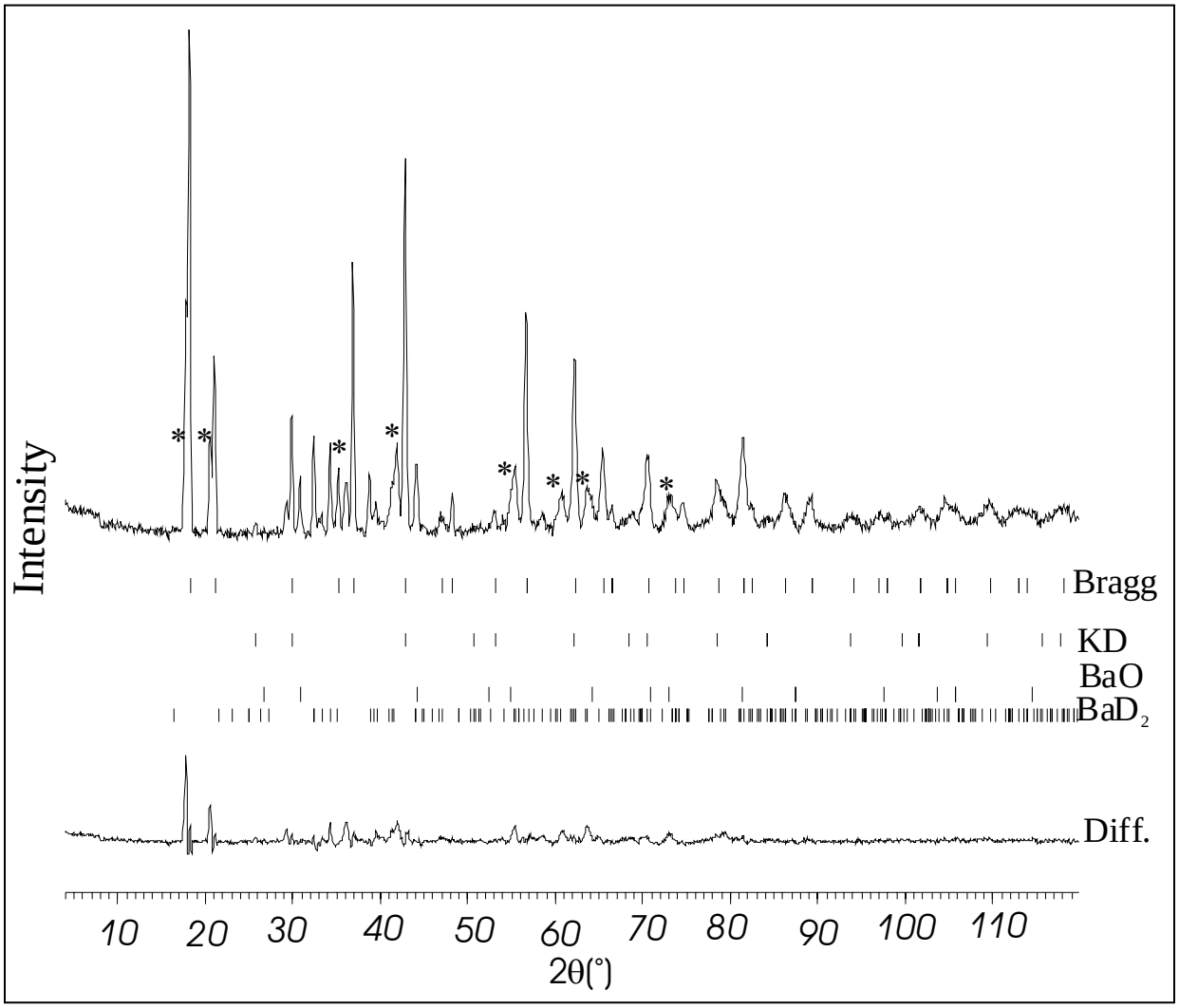

Figure 2.
The difference plot obtained in the profile refinement of the NPD data on $KBaIrD_6$. BaD_2, KD and BaO are indicated as an impurity phases. (*) indicate the second new phase (will be published in a future work).

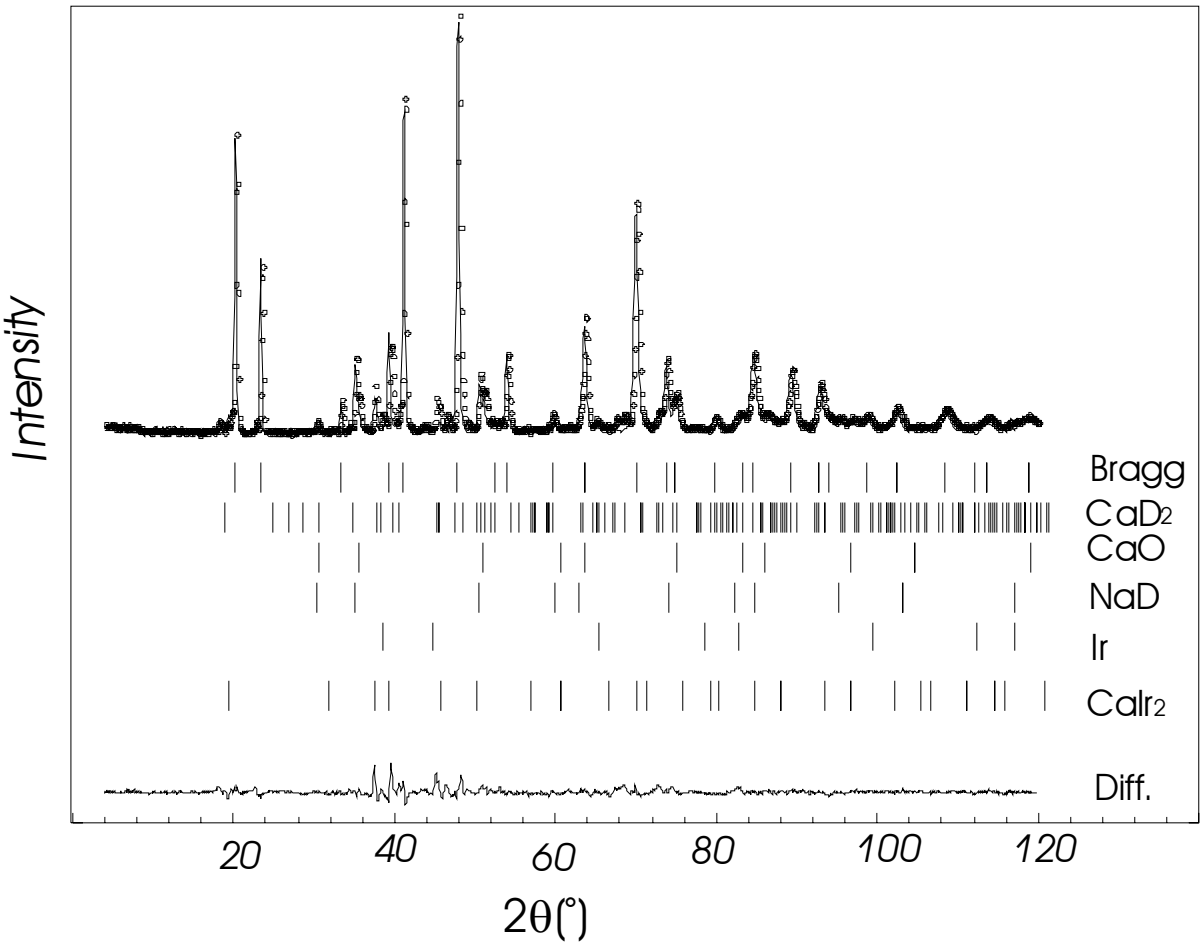

Figure 3.
The difference plot obtained in the profile refinement of the NPD data on $NaCaIrD_6$. CaD_2, CaO, NaD, Ir and $CaIr_2$ are indicated as an impurity phases.

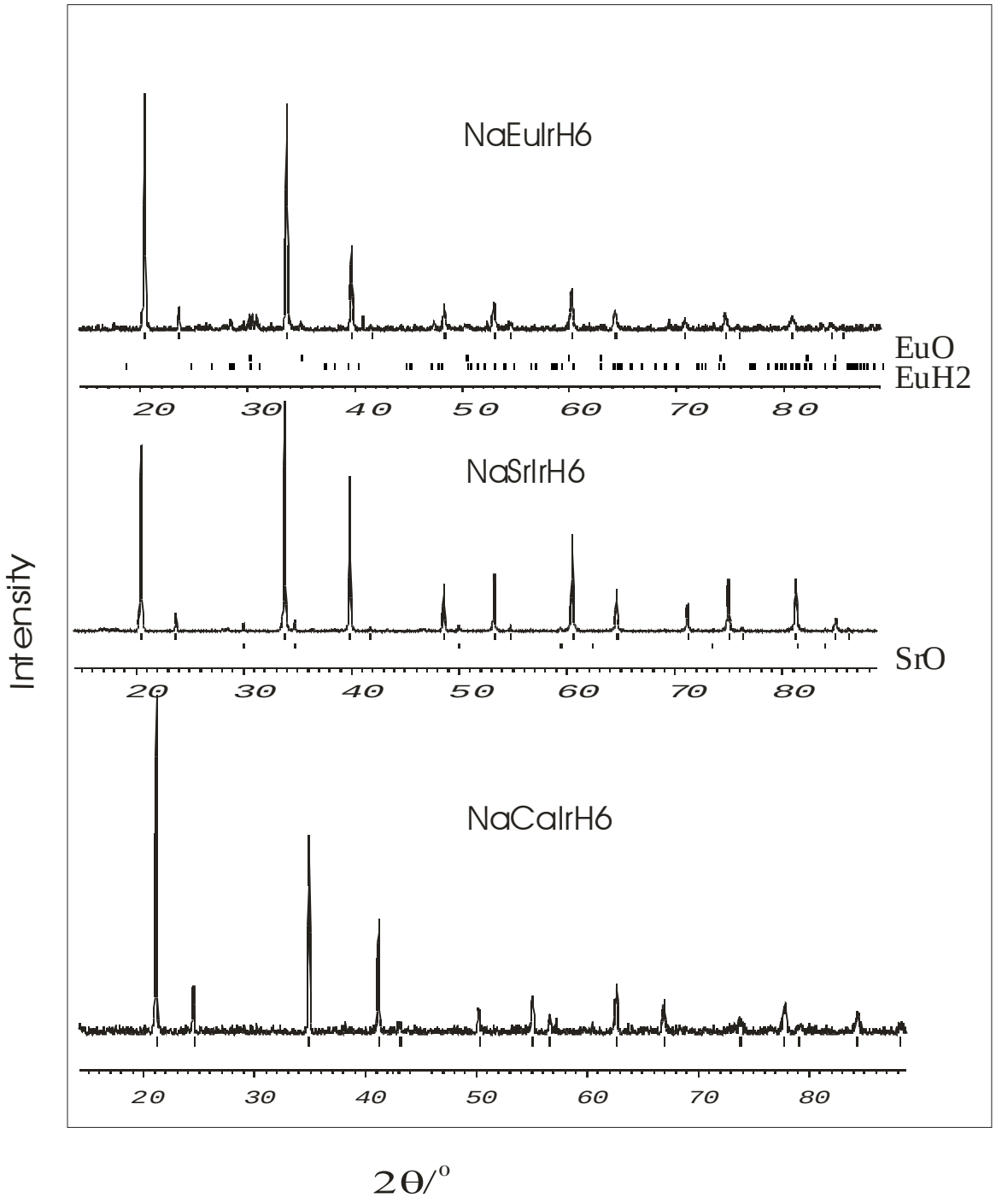

Figure 4.
Comparison of Guinier-Hägg x-ray diffraction data of $NaEuIrH_6$ and $NaSrIrH_6$ with $NaCaIrH_6$. EuO, EuH_2 and SrO are indicated as an impurity phases. Intensities versus 2θ using Cu $K\alpha_1$ radiation and with Si as the internal standard at 293K.

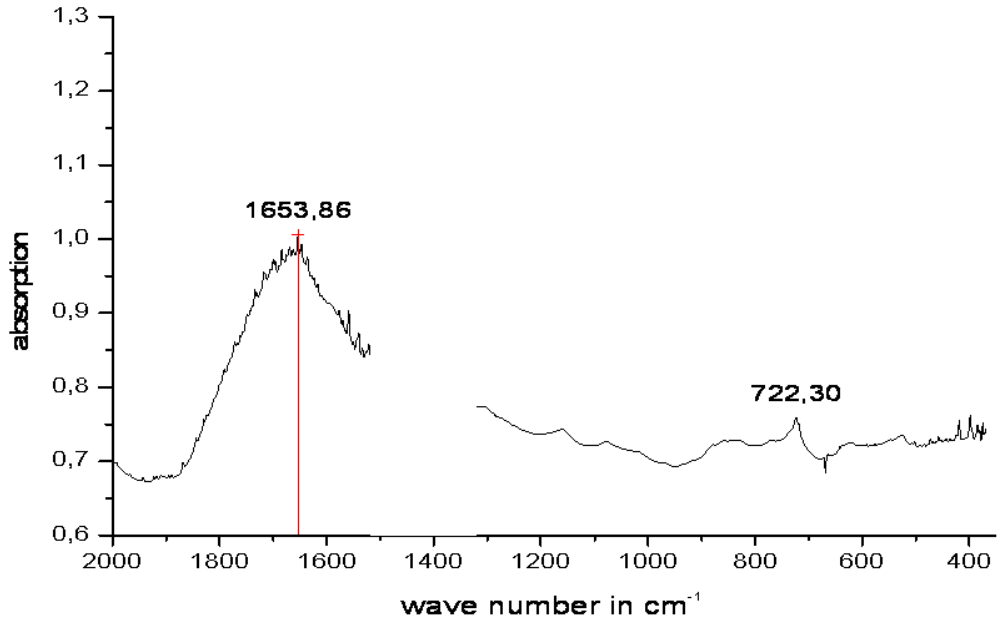

Figure 5.
Spectrum of $NaCaIrH_6$ in the range of 2000 cm^{-1} to 350 cm^{-1}. The area with the Nujol® background peaks between 1495 cm^{-1} and 1360 cm^{-1} has been removed for clarity.

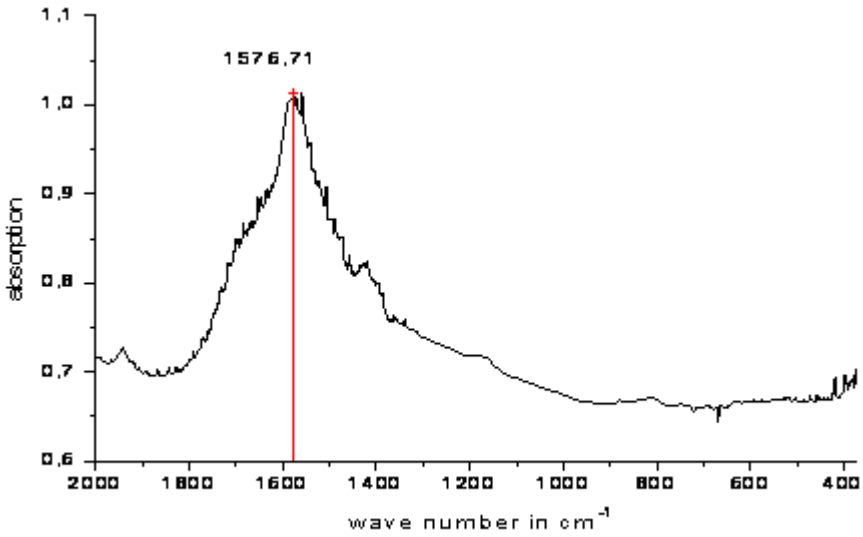

Figure 6.
Spectrum of $KBaIrH_6$ in the range of 2000 cm^{-1} to 350 cm^{-1}. The area with the Nujol® background peaks between 1495 cm^{-1} and 1360 cm^{-1} .

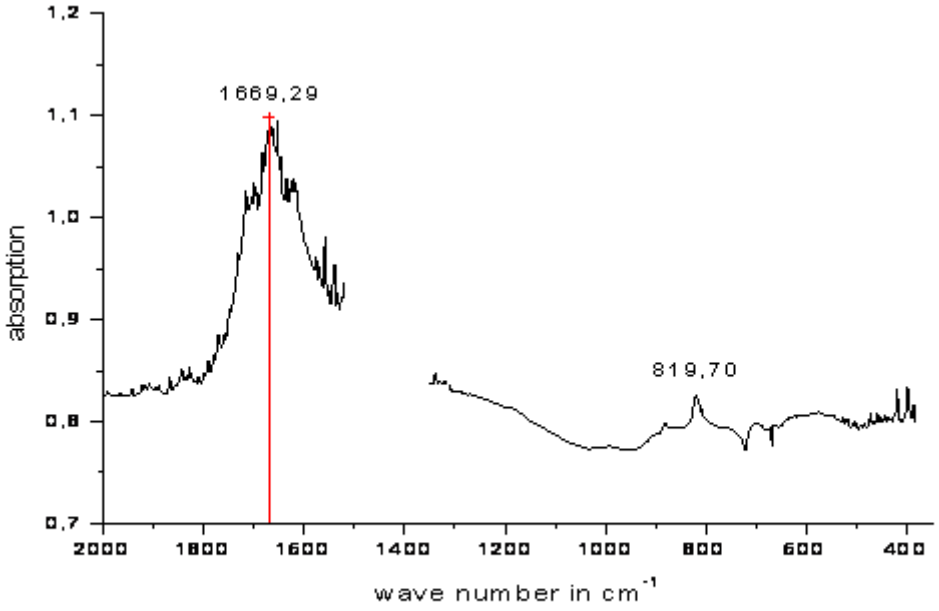

Figure 7.
Spectrum of $NaSrIrH_6$ in the range of 2000 cm^{-1} to 350 cm^{-1}. The area with the Nujol® background peaks between 1495 cm^{-1} and 1360 cm^{-1} has been removed for clarity.

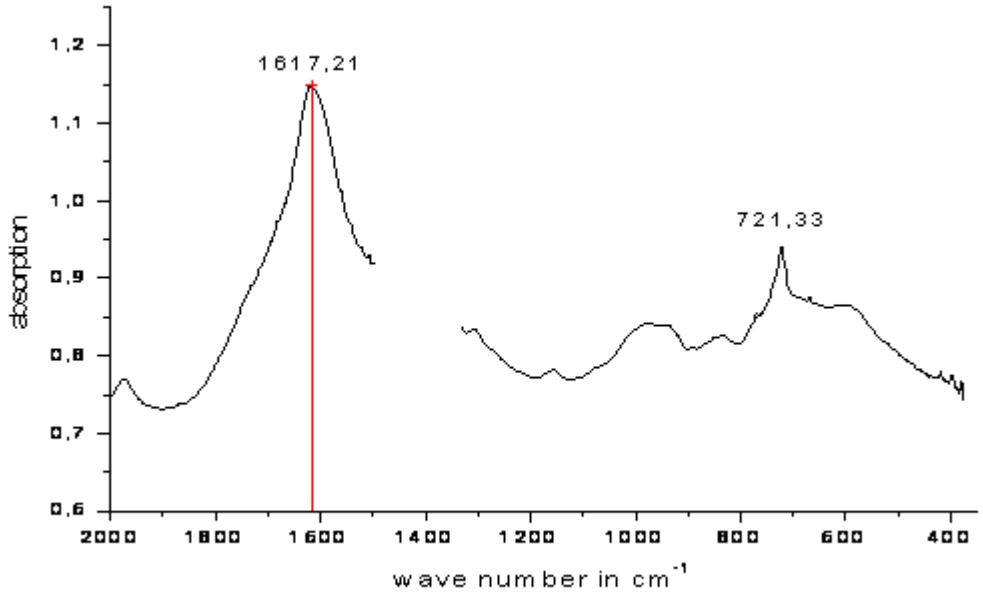

Figure 8.
Spectrum of $KSrIrH_6$ in the range of 2000 cm^{-1} to 350 cm^{-1}. The area with the Nujol® background peaks between 1495 cm^{-1} and 1360 cm^{-1} has been removed for clarity.

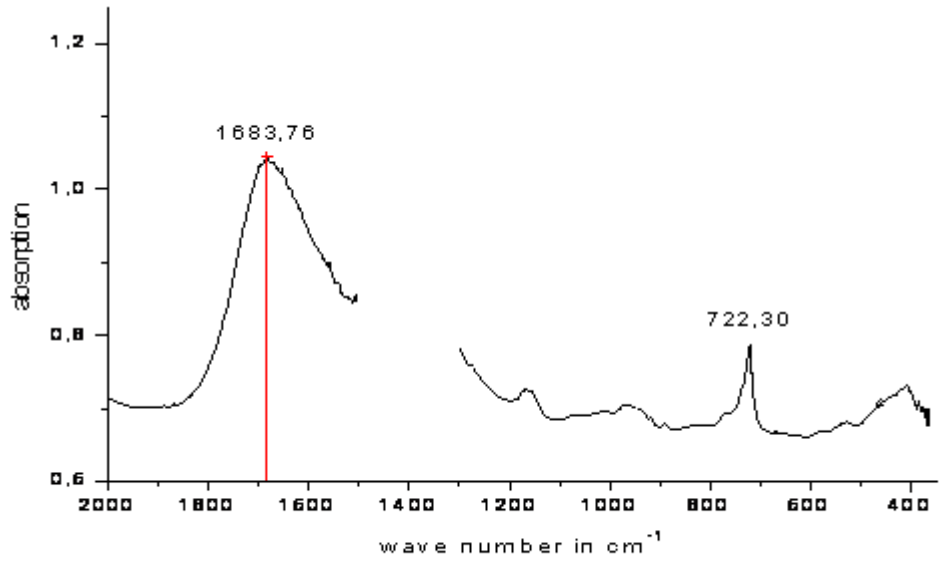

Figure 9.
Spectrum of $NaEuIrH_6$ in the range of 2000 cm^{-1} to 350 cm^{-1}. The area with the Nujol® background peaks between 1495 cm^{-1} and 1360 cm^{-1} has been removed for clarity.