

Projet ANR-12-BS05-0011

HYDRIDES

Programme **Blanc SIMIS 2012**

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A IDENTIFICATION

Acronyme du projet	HYDRIDES
Titre du projet	Excitation et chimie des hydrures interstellaires
Coordinateur du projet (société/organisme)	Alexandre Faure (IPAG)
Période du projet (date de début – date de fin)	01/01/2013 31/12/2017
Site web du projet, le cas échéant	http://ipag.osug.fr/Hydrides/

Rédacteur de ce rapport	
Civilité, prénom, nom	Alexandre Faure
Téléphone	04 76 63 55 16
Adresse électronique	alexandre.faure@univ-grenoble-alpes.fr
Date de rédaction	16/02/2018

Si différent du rédacteur, indiquer un contact pour le projet	
Civilité, prénom, nom	
Téléphone	
Adresse électronique	

Liste des partenaires présents à la fin du projet (société/organisme et responsable scientifique)	ISM Bordeaux / T. Stoecklin IPAG Grenoble / A. Faure LOMC Le Havre / F. Lique IPR Rennes / I. Sims
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B RESUME CONSOLIDE PUBLIC

B.1 INSTRUCTIONS POUR LES RESUMES CONSOLIDES PUBLICS

B.2 RESUME CONSOLIDE PUBLIC EN FRANÇAIS

HYDRIDES : Excitation et chimie des hydrures interstellaires

Contexte et objectifs : exploitation des spectres infra-rouges *Herschel*

Entre 2010 et 2013, l'observatoire spatial infra-rouge *Herschel* de l'Agence Spatiale Européenne a cartographié les hydrures¹ interstellaires avec une résolution spectrale et une sensibilité sans précédent. L'analyse fine de tels spectres a pour prérequis la connaissance des taux de collision des hydrures par H, H₂ et les électrons. Avant 2013, des données collisionnelles *précises* pour des hydrures étaient disponibles pour seulement deux espèces : HF et H₂O. Pour quelques autres hydrures, les calculs utilisaient l'atome d'hélium comme substitut à H₂, par simplicité. Or, des différences collisionnelles significatives existent entre He, H et H₂. En outre, toutes les études précédentes avaient été menées dans le cadre de l'approximation des rotateurs rigides. Cette approximation est discutable dans le cas d'ions ou de radicaux car les voies réactives avec H ou H₂ peuvent jouer un rôle, même à basse température. Les trois principaux objectifs de notre projet HYDRIDES (2013-2017) étaient *i*) d'aborder l'excitation collisionnelle de radicaux et ions hydrures avec les meilleurs outils théoriques *ii*) de comparer la théorie à l'expérience au niveau état-à-état et *iii*) d'évaluer

¹ Molécules comportant un seul atome lourd et un ou plusieurs atomes d'hydrogène, telles que CH⁺, H₂O, NH₃, etc.

l'impact des nouveaux taux de collision sur des modèles de transfert de rayonnement et de comparer les prédictions aux observations.

Méthodes : théorie quantique et expériences à basse température

Notre projet était composé de 3 tâches principales : la première tâche concernait le calcul des sections efficaces et taux de collision pour les hydrures détectés dans le milieu interstellaire. Pour mener ces calculs nous avons massivement utilisé la méthode de dynamique quantique dite *close-coupling* combinée aux meilleures surfaces d'énergie potentielle disponibles. La seconde tâche était consacrée aux mesures de laboratoire et à la comparaison entre théorie et expériences, à basse température et résolues d'état-à-état. Les techniques complémentaires de *double résonance* (en écoulements froids) et de *faisceaux moléculaires croisés* ont été mises en œuvre dans ce but. La troisième tâche s'est concentrée sur l'impact des données collisionnelles dans des modèles réalistes de transfert radiatif. Nous avons pour cela simulé les spectres observationnels à l'aide d'approches standards (probabilité d'échappement) et sophistiquées (méthodes itératives non-locales). En parallèle de ces trois tâches, nous avons développé un réseau astrochimique en phase-gaz distinguant les états de spin nucléaire des hydrures interstellaires.

Résultats majeurs du projet

1. Des données collisionnelles précises (avec H, H₂ ou les électrons) sont aujourd'hui disponibles pour une douzaine d'hydrures (sans compter les isotopologues), y compris des espèces très réactives comme CH⁺.
2. Des comparaisons théorie/expérience état-à-état pour les systèmes de référence CO+H₂ et H₂O+H₂ ont permis de valider dans le détail la grande précision des calculs quantiques dans le régime froid interstellaire (< -260 °C), proche du zéro absolu.
3. Nous avons reproduit pour la première fois quantitativement les spectres en émission des ions CH⁺ et OH⁺ mesurés par le satellite *Herschel* dans des régions de photodissociation.
4. Nous avons expliqué les rapports ortho-sur-para « anormaux » (hors équilibre) des hydrures d'azote NH₂ et NH₃ mesurés dans le milieu interstellaire. Ce développement, non prévu initialement, a ouvert la voie à l'astrochimie des spins nucléaires.

Production scientifique

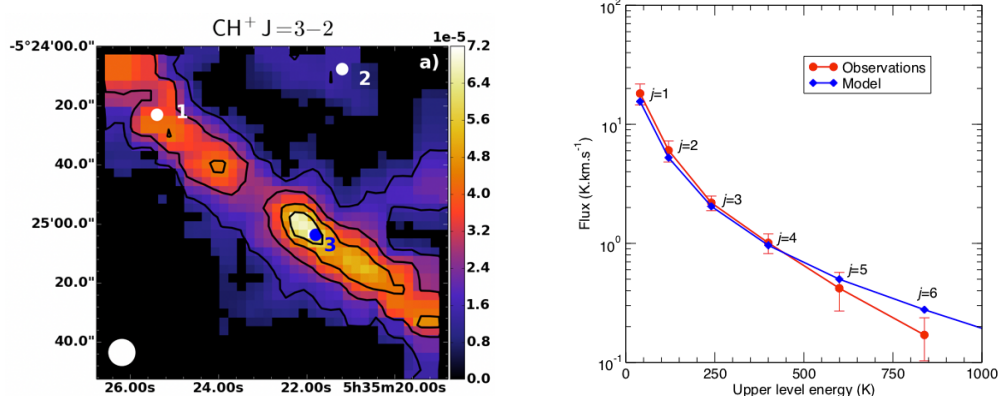
Une soixantaine d'article ont été publiés sur la période 2013-2017 dans des journaux de rang A. Parmi ces articles, on en trouve 4 publiés dans des journaux à grand facteur d'impact (Science et Nature) ainsi que 2 revues et quatre chapitres d'ouvrages. 45% des articles ont été publiés dans des journaux d'astrophysique (MNRAS, A&A, ApJ), le reste dans des journaux de physique-chimie (J. Chem. Phys., Chem. Phys. Lett. etc.). 35% des publications sont des articles inter-laboratoires. La liste complète (et les PDF) est disponible à l'adresse suivante :

<http://ipag.osug.fr/Hydrides/publications.shtml>

Les données collisionnelles (tables de fichiers textes) pour environ 30 systèmes collisionnels (en comptant les isotopologues) ont été déposées (en partie) dans les bases de données LAMDA, BASECOL et CASSIS². L'ensemble des données sera à terme mis en ligne à l'adresse <http://ipag.osug.fr/Hydrides/>.

² <http://home.strw.leidenuniv.nl/~moldata/>; <http://basecol.obspm.fr/>; <http://cassis.irap.omp.eu/?page=catalogs-collision>

Illustration



Gauche : Carte *Herschel* de l'émission de $\text{CH}^+(j=3 \rightarrow 2)$ dans la barre d'Orion (d'après Parikka et al. 2017). *Droite* : comparaison entre notre modèle d'émission de $\text{CH}^+(j \rightarrow j-1)$ et les observations *Herschel* (d'après Faure et al. 2017).

Le projet HYDRIDES est un projet de recherche fondamentale coordonné par Alexandre Faure (Institut de Planétologie et d'Astrophysique de Grenoble, IPAG). Il associe aussi l'Institut des Sciences moléculaires (ISM) de Bordeaux, le Laboratoire Ondes et Milieux Complexes (LOMC) du Havre et l'Institut de Physique de Rennes (IPR). Le projet a commencé en décembre 2013 et a duré 60 mois (prolongation de 12 mois en raison d'un incendie au laboratoire de Rennes). Il a bénéficié d'une aide ANR de 639 757 € pour un coût global de l'ordre de 5 M€.

B.3 RESUME CONSOLIDE PUBLIC EN ANGLAIS

Context and objectives: exploitation of the Herschel's infra-red spectra

In the period 2010-2013, the European Space Agency's Herschel infrared observatory has mapped interstellar hydrides³ with unprecedented spectral resolution and sensitivity. Comprehensive analysis of such spectra requires the knowledge of collisional rate coefficients for hydrides excited by H, H₂ and electrons. Before 2013, *accurate* collisional data for hydrides were available for only two species: HF and H₂O. For a few other hydrides, calculations employed the helium atom as a substitute for H₂, for simplicity. Significant collisional differences however exist between He, H and H₂. In addition, all previous studies were performed within the rigid-rotor approximation. This approximation is questionable in the case of ions or radicals because reactive channels with H or H₂ can play a role, even at low temperature. The three main objectives of the project HYDRIDES (2013-2017) were *i*) to tackle the collisional excitation of radical and ionic hydrides with the best available theoretical tools *ii*) to compare theory to experiment at the state-to-state level and *iii*) to assess the impact of the new collisional rate coefficients on radiative transfer models and to compare predictions with observations.

Methods: Quantum theory and low temperature scattering experiments

Our project was composed of three main tasks: the first task concerned the computation of collisional cross sections and rate coefficients for small hydrides detected in the interstellar medium. The so-called *close-coupling* quantum scattering theory was used massively and combined with the best available potential energy surfaces. The second task was devoted to laboratory measurements and comparisons with theoretical data, at low-temperature and state-

³ Molecules containing a single heavy atom with one or more hydrogen atoms, such as CH⁺, H₂O, NH₃, etc.

resolved. The complementary techniques of *double resonance* (in cold flows) and *crossed molecular beams* were implemented. The third and last task focused on the impact of the collisional data on realistic radiative transfer models. To this aim, we have modeled observational spectra using standard (escape probability) as well as sophisticated (non-local iterative methods) approaches. In parallel with these tasks, we have developed a gas-phase astrochemical network distinguishing the nuclear-spin states of interstellar hydrides.

Major results

1. Accurate collisional data (with H, H₂ or electrons) are now available for a dozen of hydrides (not including isotopologues), including highly reactive species such as CH⁺.
2. Comparisons between state-to-state theory and experiment for the benchmark systems CO+H₂ and H₂O+H₂ have validated in detail the high precision of quantum calculations in the cold interstellar regime (< -260 °C), near absolute zero.
3. We have quantitatively reproduced, for the first time, the emission spectrum of CH⁺ and OH⁺ as measured by *Herschel* satellite in photodissociation regions.
4. We have explained the “anomalous” (out of equilibrium) ortho-to-para ratio of nitrogen hydrides NH₂ and NH₃ in the cold interstellar medium. This development, not initially planned, has paved the way to the nuclear-spin specific astrochemistry.

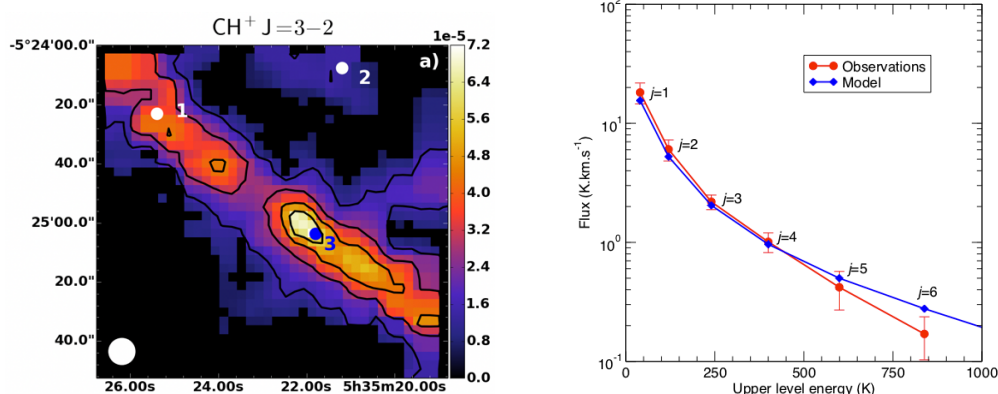
Scientific production

About 60 papers were published over the period 2013-2017 in rank “A” journals. Among these articles, 4 were published in journals with high impact factor (Science and Nature) as well as 2 reviews and four chapters in books. 45% of publications were published in astrophysical journals (MNRAS, A&A, ApJ) while the remaining publications were published in physical-chemistry journals (J. Chem. Phys., Chem. Phys. Lett., etc.). 35% of publications are inter-laboratory articles. The complete list (including PDF) is available here:

<http://ipag.osug.fr/Hydrides/publications.shtml>

Collisional data (text file tables) for about 30 collisional systems (including isotopologues) have been (partly) placed in the LAMDA, BASECOL and CASSIS databases⁴. The full set of data will be made available soon at <http://ipag.osug.fr/Hydrides/>.

Illustration



Left : *Herschel* map of the CH⁺($j=3\rightarrow 2$) emission in the Orion bar (from Parikka et al. 2017).

Right : Comparison between our emission model for CH⁺($j\rightarrow j-1$) and the *Herschel* observations (from Faure et al. 2017).

⁴ <http://home.strw.leidenuniv.nl/~moldata/>; <http://basecol.obspm.fr/>; <http://cassis.irap.omp.eu/?page=catalogs-collision>

The HYDRIDES project is a fundamental research programme coordinated by Alexandre Faure (Institut de Planétologie et d'Astrophysique de Grenoble, IPAG). It involves the Institut des Sciences moléculaires (ISM) at Bordeaux, the Laboratoire Ondes et Milieux Complexes (LOMC) at Le Havre and the Institut de Physique de Rennes (IPR). The project started in December 2013 and lasted 60 months (including a 12 months extension due to a fire in Rennes laboratory). It has received funding of 639 757 € from the ANR for a global cost of about 5 M€.

C MEMOIRE SCIENTIFIQUE

Mémoire scientifique confidentiel : non

C.1 RESUME DU MEMOIRE.

In the period 2010-2013, the European Space Agency's Herschel infrared observatory has mapped interstellar hydrides⁵ with unprecedented spectral resolution and sensitivity. The comprehensive analysis of such spectra requires the knowledge of collisional rate coefficients for hydrides excited by H, H₂ and electrons. Before 2013, *accurate* collisional data for hydrides were available for only two species: HF and H₂O. For a few other hydrides, calculations employed helium atom as a substitute for H₂, for simplicity. Significant differences however exist between He, H and H₂. In addition, all previous studies were performed within the rigid-rotor approximation. This approximation is questionable in the case of ions or radicals because reactive channels with H or H₂ can play a role, even at low temperature. The three main objectives of the project HYDRIDES (2013-2017) were *i*) to tackle the collisional excitation of radical and ionic hydrides with the best available theoretical tools *ii*) to compare theory to experiment at the state-to-state level and *iii*) to assess the impact of the new collisional rate coefficients on radiative transfer models and to compare predictions with observations.

C.2 ENJEUX ET PROBLEMATIQUE, ETAT DE L'ART

Because hydrogen is much more abundant than any other element in the interstellar medium (ISM), hydrides are the first molecules to form. They constitute significant reservoirs of heavy elements, as well as sensitive tests of interstellar chemistry networks and of the ambient physical conditions. In the period 2010-2013, the European Space Agency's Herschel infrared observatory has mapped interstellar hydrides with unprecedented spectral resolution and sensitivity (Gérin et al. 2016). Hydrides are difficult to observe from ground-based observatories because most of their transitions fall into frequency regions with strongly reduced atmospheric transmission. The comprehensive analysis of *Herschel* spectra requires the knowledge of collisional rate coefficients for hydrides excited by H, H₂ and electrons. Indeed, a general property of astronomical molecular spectra is that the populations of the energy levels are rarely at local thermodynamic equilibrium (LTE). In such conditions, interpreting a spectrum requires the simultaneous solution of the radiative transfer equation and a set of statistical equilibrium equations for the molecular energy levels. Solving the statistical equilibrium equations in turn necessitates the availability of the rate coefficients for collisional (de)excitation. Before 2013, *accurate* collisional data for hydrides were available for only HF (Guillon & Stoecklin 2012) and H₂O (Daniel et al. 2011). For a few other hydrides, calculations employed helium atom as a substitute for H₂, for simplicity (see e.g. Lanza & Lique 2012). It is now well known that significant differences exist between He, H and H₂. In addition, all previous studies were performed within the rigid-rotor approximation. This approximation, which is well adapted for neutral closed-shell species, is questionable in the case of ions or

⁵ Molecules with a single heavy atom and one or several hydrogen atoms, such as CH⁺, OH, H₂O, etc.

radicals because the reactive channels with H or H₂ can play a role, even at low temperature. The three main objectives of the project HYDRIDES (2013-2017) were *i*) to tackle the collisional excitation of radical and ionic hydrides with the best available theoretical tools *ii*) to compare theory to experiment at the state-to-state level and *iii*) to assess the impact of the new collisional rate coefficients on radiative transfer models and to compare predictions with observations. This latter objective was combined with (initially not planned) detailed gas-phase chemical modelling.

C.3 APPROCHE SCIENTIFIQUE ET TECHNIQUE

Our project was composed of three main tasks: the first task concerned the computation of collisional cross sections and rate coefficients for small hydrides detected in the interstellar medium. The so-called *close-coupling* quantum scattering theory was used massively and combined with the best available potential energy surfaces (PES). The second task was devoted to laboratory measurements and comparisons with theoretical data, at low temperature and state-to-state. The complementary techniques of *double resonance* in cold flows and *crossed molecular beams* were implemented. The third and last task focused on the impact of the new collisional data on realistic radiative transfer models. To this end, we have modeled observational spectra using standard (escape probability) as well as sophisticated (non-local iterative methods) radiative transfer methods. In parallel, we have developed a gas-phase chemical network distinguishing hydrides with nuclear-spin isomers (hydrides with several equivalent hydrogens like NH₃)

C.4 RESULTATS OBTENUS

The major theoretical and experimental results of our project are summarized in the four main points below:

1. **Accurate collisional data (with H, H₂ or electrons) have been computed for a dozen of hydrides** (not including isotopologues): CH, CH⁺, NH₂, NH₃, OH, OH⁺, H₂O, SH⁺, HF, HCl, HeH⁺, ArH⁺. These include reactive ions and radicals (with doublet and triplet electronic states), with both fine and hyperfine structures. Calculations have involved the best available PES combined with quantum scattering theories. Data have been (partly) placed in the LAMDA, BASECOL and CASSIS databases. The full set of data will be made available at <http://ipag.osug.fr/Hydrides/>.
2. **The rigid-rotor approximation was evaluated in several ways.** It was found to be extremely accurate in the case of non-reactive systems, as expected (Faure et al. 2016). In the case of reactive systems, it was found to provide reliable results at low energy provided that the reaction is endothermic or proceeds through a barrier (Stoeklin et al. 2015, Lique 2015). On the other hand, for exothermic reactions without barrier or endothermic reactions with deep potential wells, the rigid-rotor approximation was found to overestimate the inelastic cross sections by up to an order of magnitude (Bulut et al. 2015, Faure et al. 2017).
3. **The accuracy of theory was validated by state-to-state measurements** in the low temperature regime (< 50 K). The CO molecule (not a hydride) was initially investigated as a benchmark target. Measurements have involved crossed molecular beam (in Bordeaux) and double resonance (in Rennes) experiments. The former was able to probe in detail the near-threshold regime where cross sections are dominated by resonances (Chefdeville et al. 2013, 2015). The latter has measured *absolute* rate coefficients down to 5K (Mertens et al. 2017, Labiad et al. in prep.). Results were recently extended to H₂O in Bordeaux (Bergeat et al. to be submitted) and are planned for OH in Rennes.
4. **The chemistry of nuclear-spin isomers was explored** by developing a new gas-phase chemical network distinguishing the nuclear-spin states (ortho, para, meta) of multi-

hydrogenated hydrides. Our theoretical treatment consists in assuming conservation of the total nuclear spin and full scrambling of the nuclei in the reaction complex (Rist et al. 2013). This contribution to the project HYDRIDES was not initially planned.

C.5 EXPLOITATION DES RESULTATS

The collisional data computed within the HYDRIDES project were exploited in many astrophysical applications, by several international groups and also by ourselves. We give below a list of astrophysical applications led by us:

1. **Ortho-to-para ratio of ammonia in the cold diffuse ISM.** This work has demonstrated that the low ortho-to-para ratio of H₂ in the ISM drives the ortho-to-para ratios of hydrides out of statistical or thermal values (Faure et al. 2013).
2. **The chemistry of nitrogen hydrides revisited.** We have developed a new gas-phase chemical network which was able to reproduce, for the first time, the NH/NH₂/NH₃ ratios measured with *Herschel* toward a protostar (Le Gal et al. 2014).
3. **Chlorine abundance in the ISM.** The new HCl+H₂ and HCl+H rate coefficients were found to significantly increase the line intensities with respect to HCl-He rate coefficients, suggesting an even lower HCl abundance and confirming that HCl is not an important chlorine carrier in the ISM (Lanza et al. 2014, Lique & Faure 2017).
4. **Electron density in the Crab nebula.** The modeling of *Herschel* emission spectra of ArH⁺ allowed us to use this ion as a probe and to derive an electron density $n(e^-) \sim 2500 \text{ cm}^{-3}$ in the Crab nebula, as expected from supernova remnant models (Hamilton et al. 2015).
5. **Deuteration of nitrogen hydrides in prestellar cores.** Modeling of NH absorption and ND emission was carried out in Bacmann et al. (2016). The study of the D/H and ortho/para ratios of NH₃ isotopologues toward several prestellar cores was investigated in detail in Daniel et al. (2016), Harju et al. (2017) and Hily-Blant et al. (2018).
6. **Excitation of CH⁺ and OH⁺ in photodissociation regions.** The full set of inelastic and reactive data computed for CH⁺ and OH⁺ allowed us to reproduce quantitatively, for the first time, the line fluxes measured by *Herschel* toward two prototypical photodissociation regions (the Orion bar and NGC 7027), confirming the importance of chemical pumping in the case of CH⁺ and providing further evidence for vibrationally excited H₂ in these sources (Faure et al. 2017, Hamilton et al. 2018).
7. **New calibration of the NH₃ thermometer.** Collisional rate coefficients for NH₃ excited by pH₂, oH₂ and H were used to calibrate the ammonia thermometer with high precision for each collider (Bouhafs et al. 2017).

C.6 DISCUSSION

All the main objectives of the project HYDRIDES were achieved, including the most challenging ones. Theoretically, converging close-coupling calculations for strongly bound complexes (such as CH₂⁺ and OH₂⁺) is a major step forward. These calculations have no equivalent in the literature and they were considered as highly risky in the original proposal. Experimentally, the measurement of *absolute* state-to-state inelastic rate coefficients at temperatures as low as 5K is a major breakthrough. The complementary but challenging objective of directly observing resonances in inelastic collisions, as predicted by theory, was successfully completed as well. Theoretical and experimental results were obtained with H or H₂ *and not He* as a projectile, which is a significant advance. Finally, the implementation of the new collisional data in radiative transfer models has provided relevant astrophysical results (see above).

These different results place our laboratories at the forefront of molecular excitation studies for astrophysics. The next natural challenge is the extension of our calculations to tetratomic, pentatomic and even larger reactive systems such as CH^+H_2 and $\text{H}_2\text{O}^+\text{H}_2$. The CH_3^+ PES has been recently determined in Bordeaux but scattering calculations are currently only possible with approximate methods (statistical or classical) due to the computational cost of close-coupling calculations. These alternative methods now need to be fully tested. Finally, in addition to their role in molecular energy transfer, such reactive collisions (involving hydrogen atom exchanges) are crucial to model the nuclear-spin chemistry of hydrides and to predict reliable ortho-to-para ratios.

C.7 CONCLUSIONS

The HYDRIDES project is without any doubt a success story. The three key objectives *i)* computing collisional data for reactive hydrides *ii)* comparing theory to low temperature state-resolved experiments and *iii)* assessing the impact of the new data on astrophysical models were all achieved and, in some cases, exceeded. In particular, HYDRIDES has paved the way to a new class of astrophysical probes: the reactive molecules. At the same time, a new era has begun with molecular excitation calculations that involve strongly bound complexes for which conventional methods are severely limited by the computational cost. The need for new theoretical methods is evident. These developments should be accompanied by new experiments also devoted to reactive species. Our experience with HYDRIDES is a major asset on which to build. The knowledge we have gained gives us confidence to undertake even more ambitious projects that will enable the consortium partners to consolidate their leading position in the domain of molecular excitation studies for astrophysics.

C.8 REFERENCES

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D LISTE DES LIVRABLES

Date de livraison	N°	Titre	Nature (rapport, logiciel, prototype, données, ...)	Partenaires (souligner le responsable)	Commentaires
2015-2018	1	CO excitation by H ₂	Crossed beam and CRESU measurements	Bordeaux (Costes) and Rennes (Sims)	Benchmark system
2015	2	CH excitation by He	Theoretical data	Le Havre (Lique)	
-	2	CH excitation by H ₂	Theoretical data	Le Havre (Lique)	Cancelled (done in Baltimore)
-	2	CH excitation by He/H ₂	CRESU measurements	Rennes (Sims)	Cancelled
2016	2	OH excitation by He	Theoretical data	Le Havre (Lique)	
2017	2	OH excitation by H ₂	Theoretical data	Le Havre (Lique) and Grenoble (Faure)	
-	2	OH excitation by H ₂	Crossed beam and CRESU measurements	Bordeaux (Costes) and Rennes (Sims)	Crossed beam cancelled (done in Nijmegen). CRESU in progress
-	3	CH, OH and NH excitation by H	Theoretical data	Le Havre (Lique)	Cancelled
2017	4	CH ⁺ excitation by H	Theoretical data	Bordeaux (Stoecklin)	
-	4	CH ⁺ excitation by H ₂	Theoretical data	Bordeaux (Stoecklin)	In progress
2017	4	CH ⁺ excitation by e ⁻	Theoretical data	Grenoble (Faure)	
2017	4	CH ⁺ dissociative recombination	Theoretical data	Le Havre (Schneider)	
-	5	CH, NH, OH radiative transfer	Model	Grenoble (Faure)	Cancelled
2017	5	Coupled radiative transfer/chemical code	Code	Grenoble (Faure)	Extension of the public code RADEX
2017	5	CH ⁺ radiative transfer	Model	Grenoble (Faure)	
2016		OH ⁺ excitation by He, H	Theoretical data	Le Havre (Lique)	Not planned
2016-2018		OH ⁺ , SH ⁺ , HeH ⁺ , ArH ⁺ excitation by e ⁻	Theoretical data	Grenoble (Faure)	Not planned
2014		HCl excitation by H, H ₂ , e ⁻	Theoretical data	Le Havre (Lique) and Grenoble (Faure)	Not planned
2015		H ₂ O excitation by H	Theoretical data	Grenoble (Daniel)	Not planned
2017		H ₂ O excitation by H ₂	Crossed beam measurements	Bordeaux (Bergeat)	Not planned
2018		D ₂ O excitation by H ₂	Crossed beam measurements	Bordeaux (Bergeat)	Not planned
2017		NH ₂ excitation by H ₂	Theoretical data	Le Havre (Lique) and Grenoble (Faure)	Not planned
2017		NH ₃ excitation by H	Theoretical data	Le Havre (Lique) and Grenoble (Faure)	Not planned
2016		NH ₂ D, NHD ₂ and ND ₃ excitation by H ₂	Theoretical data	Grenoble (Daniel)	Not planned
2018		Nuclear-spin chemical network	Chemical network	Grenoble	Not planned

E IMPACT DU PROJET

E.1 INDICATEURS D'IMPACT

Nombre de publications et de communications (à détailler en E.2)

		Publications multipartenaires	Publications monopartenaires
International	Revue à comité de lecture	20	35
	Ouvrages ou chapitres d'ouvrage	1	4

	Communications (conférence)	~15 invited lectures	~15 invited lectures
France	Revue à comité de lecture		
	Ouvrages ou chapitres d'ouvrage		
	Communications (conférence)		
Actions de diffusion	Articles vulgarisation	1	3
	Conférences vulgarisation	1	
	Autres		

Autres valorisations scientifiques (à détailler en 0)

	Nombre, années et commentaires (valorisations avérées ou probables)
Brevets internationaux obtenus	
Brevet internationaux en cours d'obtention	
Brevets nationaux obtenus	
Brevet nationaux en cours d'obtention	
Licences d'exploitation (obtention / cession)	
Créations d'entreprises ou essaimage	
Nouveaux projets collaboratifs	1 (projet PICS Le Havre – Grenoble- Madrid 2018-2021)
Colloques scientifiques	3 (Atelier St Florent "Hydrures" 2015, Nuclear-spin workshop Grenoble 2017, Hydride workshop Telluride 2018)
Autres (préciser)	

E.2 LISTE DES PUBLICATIONS ET COMMUNICATIONS

The complete list (including PDF) of rank "A" publications (total 55) is available here: <http://ipag.osug.fr/Hydrures/publications.shtml>

The three partners in Bordeaux (Naulin, Bergeat), Le Havre (Lique) and Rennes (Sims, Le Picard) have written three chapters in the book "*Cold chemistry: molecular scattering and reactivity near absolute zero*" edited by Olivier Dulieu and Andreas Osterwalder (publisher: Royal Society of Chemistry, December 2017). The two partners in Grenoble (Faure) and Le Havre (Lique) are also editors of the book "*Gas phase chemistry in space: from elementary particles to complex organic molecules*" to be published by IOP ebooks (2018).

Finally, all consortium partners have also presented their work at several national and international conferences, through invited and contributed talks. Two illustrative examples are the international conference "The Hydride toolbox" held in Paris in December 2016 (<https://hydride-toolbox.sciencesconf.org/program>) and the international workshop "Hydride chemistry: from Earth to space" to be held in Telluride (USA) in March 2018 (<https://www.telluridescience.org/meetings/workshop-details?wid=631>) where respectively 4 (over 50 speakers) and 6 (over 22 speakers) members from the consortium have presented invited or contributed talks.

LISTE DES ÉLÉMENTS DE VALORISATION

In addition to our contributions to many conferences, we have ourselves organized three important workshops related to hydride chemistry:

1. In June 2015, we organized a national workshop on “Chimie et excitation des hydrures” held in St Florent (Corse, SOC: Lique & Faure). The scientific program can be found here: <http://ipag.osug.fr/StFlorent/2015.shtml>
2. In May 2017, we organized an international workshop on “Nuclear spin effects in astrochemistry” held in Grenoble (SOC: Faure & Hily-Blant). Full details can be found here: <https://nuclearspin2017.sciencesconf.org/>
3. In March 2018, we are co-organizing an international workshop on “Hydride chemistry: from earth to space” to be held in Telluride (USA, SOC: Lique, Neufeld & Alexander). Full details can be found here: <https://www.telluridescience.org/meetings/workshop-details?wid=631>

Finally, a « Projet International de Coopération Scientifique » (PICS) submitted to the CNRS in June 2017 by F. Lique was recently accepted for funding. This project called CEHISM (“Collisional excitation of hydrides in the interstellar medium”) will be carried out between Le Havre (PI F. Lique), Grenoble (A. Faure, P. Hily-Blant) and Madrid (CSIC, PI O. Roncero) and will combine theoretical calculations with radiative transfer models. It is funded for 3 years (15 k€ for meetings and conferences).

E.3 BILAN ET SUIVI DES PERSONNELS RECRUTES EN CDD (HORS STAGIAIRES)

Identification				Avant le recrutement sur le projet			Recrutement sur le projet				Après le projet				
Nom et prénom	Sexe H/F	Adresse email (1)	Date des dernières nouvelles	Dernier diplôme obtenu au moment du recrutement	Lieu d'études (France, UE, hors UE)	Expérience prof. Antérieure, y compris post-docs (ans)	Partenaire ayant embauché la personne	Poste dans le projet (2)	Durée missions (mois) (3)	Date de fin de mission sur le projet	Devenir professionnel (4)	Type d'employeur (5)	Type d'emploi (6)	Lien au projet ANR (7)	Valorisation expérience (8)
Kalugina Yulia	F	yulia.kalugina@gmail.com	11/2017	PhD	Hors UE	3 (thèse) +2	Le Havre (LOMC)	Post-doc	10	11/2013	Post-doc étranger	Recherche publique	Chercheur	Non	oui
Alpizar Otoniel	H	otonieldenisalpizar@gmail.com	05/2017	PhD	Hors UE	3 (thèse)	Bordeaux (ISM)	Post-doc	12	09/2015	CDI	Recherche publique	Chercheur	Non	oui
Fourmier Martin	H	fournier.martin@gmail.com	12/2017	PhD	France	3 (thèse)	Rennes (IPR)	Post-doc	12	12/2015	Post-doc étranger	Recherche publique	Chercheur	Non	oui
Labiad Hamza	H	hamza.labiad@univ-rennes1.fr	02/2018	Master 2	France	0	Rennes (IPR)	PhD	36	12/2017	Post-doc France	Recherche publique	Chercheur	Oui	oui
Daniel Fabien	H	fabien128@gmail.com	12/2017	PhD	France	3 (thèse) +5	Grenoble (IPAG)	Post-doc	24	02/2016	CDI	Privé	Ingénieur	Non	non

Aide pour le remplissage

- (1) **Adresse email** : indiquer une adresse email la plus pérenne possible
- (2) **Poste dans le projet** : post-doc, doctorant, ingénieur ou niveau ingénieur, technicien, vacataire, autre (préciser)
- (3) **Durée missions** : indiquer en mois la durée totale des missions (y compris celles non financées par l'ANR) effectuées sur le projet
- (4) **Devenir professionnel** : CDI, CDD, chef d'entreprise, encore sur le projet, post-doc France, post-doc étranger, étudiant, recherche d'emploi, sans nouvelles
- (5) **Type d'employeur** : enseignement et recherche publique, EPIC de recherche, grande entreprise, PME/TPE, création d'entreprise, autre public, autre privé, libéral, autre (préciser)
- (6) **Type d'emploi** : ingénieur, chercheur, enseignant-chercheur, cadre, technicien, autre (préciser)
- (7) **Lien au projet ANR** : préciser si l'employeur est ou non un partenaire du projet
- (8) **Valorisation expérience** : préciser si le poste occupé valorise l'expérience acquise pendant le projet.

Les informations personnelles recueillies feront l'objet d'un traitement de données informatisées pour les seuls besoins de l'étude anonymisée sur le devenir professionnel des personnes recrutées sur les projets ANR. Elles ne feront l'objet d'aucune cession et seront conservées par l'ANR pendant une durée maximale de 5 ans après la fin du projet concerné. Conformément à la loi n° 78-17 du 6 janvier 1978 modifiée, relative à l'Informatique, aux Fichiers et aux Libertés, les personnes concernées disposent d'un droit d'accès, de rectification et de suppression des données personnelles les concernant. Les personnes concernées seront informées directement de ce droit lorsque leurs coordonnées sont renseignées. Elles peuvent exercer ce droit en s'adressant l'ANR (<http://www.agence-nationale-recherche.fr/Contact>).