

Lista de publicaciones por año.

Grupo de Cinética y Dinámica de las Reacciones Químicas UR – UB.

Lista de publicaciones. Actualizada hasta junio 2012.

2012

A. Tomić, M. González, S. Tomić

The large scale conformational change of the human DPP III-substrate prefers the “closed” form
Journal of Chemical Information and Modeling 52, 1583–1594 (2012)

R. Martínez, P.A. Enríquez, M.P. Puyuelo, M. González

Dynamics of the $O(^3P) + CH_4 \rightarrow OH + CH_3$ reaction is similar to that of a triatomic reaction
Journal of Physical Chemistry A 116, 5026–5029 (2012)

2011

M. González, J. Mayneris-Perxachs, A. Saracibar, E. García

Capture and dissociation in the complex-forming $CH(v = 0,1) + D_2 \rightarrow CHD + D$, $CD_2 + H$, $CD + HD$ reactions and comparison with $CH(v = 0,1) + H_2$
Physical Chemistry Chemical Physics, 13, 13638–13644 (2011)

P. Gamallo, P. Defazio, M. González

Time dependent quantum dynamics study of the $Ne + H_2^+(v_0 = 0-4, j_0 = 1) \rightarrow NeH^+ + H$ proton transfer reaction, including the Coriolis coupling. A system with oscillatory cross sections
Journal of Physical Chemistry A 115, 11525–11530 (2011)

J.D. Sierra, L. Bonnet, M. González

Quasi-classical trajectory-Gaussian binning study of the $OH + D_2 \rightarrow HOD(v_1', v_2', v_3') + D$ angle-velocity and vibrational distributions at a collision energy of 0.28 eV
Journal of Physical Chemistry A 115, 7413–7417 (2011)

M. González, A. Saracibar, E. García

Capture and dissociation in the complex-forming $CH + H_2 \rightarrow CH_2 + H$, $CH + H_2$ reactions
Physical Chemistry Chemical Physics 13, 3421–3428 (2011)

M. González, A. Rodríguez, R. Martínez

Computational chemistry - A useful tool in the fight against hepatitis C
European Infectious Diseases 5, 38–43 (2011)

2010

P. Defazio, P. Gamallo, M. González, C. Petrongolo

Renner-Teller quantum dynamics of the $\text{NH}(\text{a}^1\Delta) + \text{H}$ reactions on the $\text{NH}_2 \text{A}^2\text{A}_1$ and X^2B_1 coupled surfaces
Journal of Physical Chemistry A 114, 9749-9754 (2010)

A. Rodríguez, C. Oliva, M. González

A comparative QM/MM study of the reaction mechanism of the hepatitis C virus NS3/NS4A protease with the three main natural substrates

Physical Chemistry Chemical Physics 12, 8001-8015 (2010)

P. Gamallo, R. Martínez, R. Sayós, M. González

Quasiclassical dynamics and kinetics of the $\text{N} + \text{NO} \rightarrow \text{N}_2 + \text{O}$, $\text{NO} + \text{N}$ atmospheric reactions
Journal of Chemical Physics 132, 144304-1/-9 (2010)

P. Defazio, P. Gamallo, M. González, S. Akpınar, B. Bussery-Honvault, P. Honvault, C. Petrongolo

Quantum dynamics of the $\text{C}(\text{^1D}) + \text{HD}$ and $\text{C}(\text{^1D}) + \text{n-D}_2$ reactions on the $\tilde{\text{a}}^1\text{A}'$ and $\text{b}^1\text{A}''$ surfaces
Journal of Chemical Physics 132, 104306-1/-8 (2010)

2009

J.D. Sierra, R. Martínez, J. Hernando, M. González

The $\text{OH} + \text{D}_2 \rightarrow \text{HOD} + \text{D}$ angle-velocity distribution: Quasi-classical trajectory calculations on the YZCL2 and WSLFH potential energy surfaces and comparison with experiments at $E_{\text{T}} = 0.28 \text{ eV}$
Physical Chemistry Chemical Physics 113, 11520-11527 (2009)

J. Mayneris-Perxachs, M. González

Time-dependent quantum dynamics study of the $\text{Ne} + \text{H}_2^+(\text{v}=0-9)$ and $\text{D}_2^+(\text{v}=0-12)$ proton transfer reactions at thermal collision energies
Journal of Physical Chemistry A 113, 4105-4109 (2009)

2008

P. Gamallo, P. Defazio, M. González, C. Petrongolo

Renner-Teller coupled-channel dynamics of the $\text{N}(\text{^2D}) + \text{H}_2$ reaction and the role of the $\text{NH}_2 \text{A}^2\text{A}_1$ electronic state
Journal of Chemical Physics 129, 244307-1/-5 (2008)

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J. Mayneris, M. González, S. K. Gray

Real wavepacket code for $ABC + D \rightarrow AB + CD$ reactive scattering

Computer Physics Communications 179, 741-747 (2008)

J. Mayneris, J. D. Sierra, M. González

Time dependent quantum dynamics study of the $Ne + H_2^+(v=0-4) \rightarrow NeH^+ + H$ proton transfer reaction

Journal of Chemical Physics, 128, 194307-1/-8 (2008)

J. Mayneris, R. Martínez, J. Hernando, S.K. Gray, M. González

Quantum dynamics study of the $K + HF(v=0-2, j=0) \rightarrow KF + H$ reaction and comparison with quasiclassical trajectory results

Journal of Chemical Physics 128, 144302-1/-7 (2008)

2007

A. Rodríguez, C. Oliva, M. González, M. van der Kamp, A.J. Mulholland

Comparison of different quantum mechanical/molecular mechanics boundary treatments in the reaction of the hepatitis C virus NS3 protease with the NS5A/5B substrate

Journal of Physical Chemistry B 111, 12909-12915 (2007)

R. Martínez, M. González, P. Defazio, C. Petrongolo

Searching for resonances in the reaction $Cl + CH_4 \rightarrow HCl + CH_3$: Quantum versus quasiclassical dynamics and comparison with experiments

Journal of Chemical Physics 127, 104302-1/-8 (2007)

C. Oliva, A. Rodríguez, M. González, W. Yang

A quantum mechanics/molecular mechanics study of the reaction mechanism of the hepatitis C virus NS3 protease with the NS5A/5B substrate

Proteins 66, 444-455 (2007)

2006

R. Martínez, J.D. Sierra, S.K. Gray, M. González

Time dependent quantum dynamics study of the $O^+ + H_2(v=0, j=0) \rightarrow OH^+ + H$ ion-molecule reaction and isotopic variants (D_2 , HD)

Journal of Chemical Physics 125, 164305-1/-7 (2006)

Lista de publicaciones por año.

P. Gamallo, R. Sayós, M. González, C. Petrongolo, P. Defazio

Quantum real wave-packet dynamics of the $\text{N}(^4\text{S}) + \text{NO}(X^2\Pi) \rightarrow \text{N}_2(X^1\Sigma_g^+) + \text{O}(^3\text{P})$ reaction on the ground and first excited triplet potential energy surfaces: Rate constants, cross sections, and product distributions
Journal of Chemical Physics 124, 174303-1/-11 (2006)

J. Mayneris, A. Saracibar, E.M. Golfeld, M. González, E. García, S.K. Gray

Theoretical study of the complex forming $\text{CH} + \text{H}_2 \rightarrow \text{CH}_2 + \text{H}$ reaction
Journal of Physical Chemistry A 110, 5542-5548 (2006)

R. Martínez, J.M. Lucas, X. Giménez, A. Aguilar, M. González

Exact quantum dynamics study of the $\text{O}^+ + \text{H}_2(v=0, j=0) \rightarrow \text{OH}^+ + \text{H}$ ion-molecule reaction and comparison with quasiclassical trajectory calculations
Journal of Chemical Physics 124, 144301-1/-9 (2006)

2005

R. Martínez, J.D. Sierra, M. González

Cross sections of the $\text{O}^+ + \text{H}_2 \rightarrow \text{OH}^+ + \text{H}$ ion-molecule reaction and isotopic variants (D_2 , HD): Quasiclassical trajectory study and comparison with experiments
Journal of Chemical Physics 123, 174312-1/-7 (2005)

P. Defazio, C. Petrongolo, P. Gamallo, M. González

Product distributions, rate constants, and mechanisms of the $\text{LiH} + \text{H}$ reactions
Journal of Chemical Physics 122, 214303-1/-9 (2005)

2004

J.D. Sierra, P.A. Enríquez, D. Troya, M. González

A QCT study of the cross-section, energy and angular distributions of the $\text{OH} + \text{D}_2 \rightarrow \text{HOD} + \text{D}$ reaction at $E_T=0.28$ eV on the YZCL2 surface
Chemical Physics Letters 399, 527-533 (2004)

D. Troya, J. Millán, I. Baños, M. González

Ab initio potential energy surface, variational transition state theory, and quasiclassical trajectory studies of the $\text{F} + \text{CH}_4 \rightarrow \text{HF} + \text{CH}_3$ reaction
Journal of Chemical Physics 120, 5181-5191 (2004)

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R. Martínez, J. Millán, M. González

Ab initio analytical potential energy surface and quasiclassical trajectory study of the $O^+(^4S) + H_2(X^1\Sigma_g^+) \rightarrow OH^+(X^3\Sigma^-) + H(^2S)$ reaction and isotopic variants

Journal of Chemical Physics 120, 4705-4714 (2004)

2003

I. Miquel, J. Hernando, R. Sayós, M. González

Influence of collision energy on the $N(^2D) + O_2 \rightarrow O(^3P) + NO$ reaction dynamics: A quasiclassical trajectory study involving four potential energy surfaces

Journal of Chemical Physics 119, 10040-10047 (2003)

J. Hernando, J. Millán, R. Sayós, M. González

Ab initio study of the $O(^1D) + CH_4(X^1A_1) \rightarrow OH(X^2\Pi) + CH_3(X^2A_2'')$ reaction: Ground and excited potential energy surfaces

Journal of Chemical Physics 119, 9504-9512 (2003)

P. Gamallo, M. González, R. Sayós, C. Petrongolo

Quantum wave packet dynamics of the $1^3A'' N(^4S) + NO(X^2\Pi) \rightarrow N_2(X^1\Sigma_g^+) + O(^3P)$ reaction

Journal of Chemical Physics 119, 7156-7162 (2003)

J. Hernando, R. Sayós, M. González

A QCT study of the microscopic mechanisms proceeding via the ground PES of the $O(^1D) + H_2(X^1\Sigma_g^+) \rightarrow OH(X^2\Pi) + H(^2S)$ reaction

Chemical Physics Letters 380, 123-134 (2003)

P. Gamallo, M. González, R. Sayós

Ab initio derived analytical fits of the two lowest triplet potential energy surfaces and theoretical rate constants for the $N(^4S) + NO(X^2\Pi)$ system

Journal of Chemical Physics 119, 2545-2556 (2003)

P. Gamallo, M. González, R. Sayós

Ab initio study of the two lowest triplet potential energy surfaces involved in the $N(^4S) + NO(X^2\Pi)$ reaction

Journal of Chemical Physics 118, 10602-10610 (2003)

I. Miquel, M. González, R. Sayós, G.G. Balint-Kurti, S.K. Gray, E.M. Goldfield

Quantum reactive scattering calculations of cross sections and rate constants for the $N(^2D) + O_2(X^3\Sigma_g^-) \rightarrow O(^3P) + NO(X^2\Pi)$ reaction

Journal of Chemical Physics 118, 3111-3123 (2003)

2002

D. Troya, J. Millán, I. Baños, M. González

Ab initio, kinetics and dynamics study of $\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$

Journal of Chemical Physics 117, 5730-5741 (2002)

P. Defazio, C. Petrongolo, C. Oliva, M. González, R. Sayós

Quantum dynamics of the $\text{N}(^4\text{S}) + \text{O}_2$ reaction on the $\text{X}^2\text{A}'$ and $\text{a}^4\text{A}'$ surfaces: Reaction probabilities, cross sections, rate constants, and product distributions

Journal of Chemical Physics 117, 3647-3655 (2002)

D. Troya, M.J. Lakin, G.C. Schatz, L.B. Harding, M. González

Quasiclassical trajectory study of energy and angular distributions for the $\text{H} + \text{CO}_2 \rightarrow \text{OH} + \text{CO}$ reaction

Journal of Physical Chemistry B 106, 8148-8160 (2002)

M. González, I. Miquel, R. Sayós

Ab initio, VTST, and QCT study of the $3^2\text{A}'$ potential energy surface implied in the $\text{N}(^2\text{D}) + \text{O}_2(\text{X}^3\Sigma_g^-) \rightarrow \text{O}(^3\text{P}) + \text{NO}(\text{X}^2\Pi)$ reaction

Chemical Physics Letters 360, 521-533 (2002)

R. Sayós, C. Oliva, M. González

The lowest doublet and quartet potential energy surfaces involved in the $\text{N}(^4\text{S}) + \text{O}_2$ reaction. II. *Ab initio* study of the C_{2v} -symmetry insertion mechanism

Journal of Chemical Physics 117, 680-692 (2002)

R. Sayós, C. Oliva, M. González

New analytical ($^2\text{A}'$, $^4\text{A}'$) surfaces and theoretical rate constants for the $\text{N}(^4\text{S}) + \text{O}_2$ reaction

Journal of Chemical Physics 117, 670-679 (2002)

M. González, R. Valero, R. Sayós

Ab initio and kinetics study of the ground $^1\text{A}''$ potential energy surface of the $\text{O}(^1\text{D}) + \text{N}_2\text{O} \rightarrow 2\text{NO}$, $\text{N}_2 + \text{O}_2(\text{a}^1\Delta_g)$ reactions

Chemical Physics Letters 355, 123-132 (2002)

R. Sayós, J. Hernando, M.P. Puyuelo, P.A. Enríquez, M. González

Influence of collision energy on the dynamics of the reaction $\text{O}(^1\text{D}) + \text{CH}_4(\text{X}^1\text{A}_1) \rightarrow \text{OH}(\text{X}^2\Pi) + \text{CH}_3(\text{X}^2\text{A}_2'')$

Physical Chemistry Chemical Physics 4, 288-294 (2002)

2001

M. González, I. Miquel, R. Sayós

Ab initio, VTST, and QCT study of the $1^2A''$ potential energy surface of the $N(^2D) + O_2(X^3\Sigma_g^-) \rightarrow O(^3P) + NO(X^2\Pi)$ reaction

Journal of Chemical Physics 115, 8838-8851 (2001)

R. Sayós, C. Oliva, M. González

Ab initio CASPT2//CASSCF study of the $O(^1D) + H_2O(X^1A_1)$ reaction

Journal of Chemical Physics 115, 8828-8837 (2001)

R. Sayós, J. Hernando, J.D. Sierra, M.A. Rodríguez, M. González

Ab initio ground PES and QCT study of the influence of molecular alignment and vibrational excitation on the $K + HF \rightarrow KF + H$ reaction

Physical Chemistry Chemical Physics 3, 4701-4711 (2001)

M. González, M.P. Puyuelo, J. Hernando, R. Sayós, P.A. Enríquez, J. Guallar

Influence of collision energy on the nascent $OH(X^2\Pi, v''=0-4)$ product energetics for the reaction of $O(^1D)$ with ethane. A laser-induced fluorescence and quasiclassical trajectory study

Journal of Physical Chemistry A 105, 9834-9844 (2001)

M. González, R. Valero, J.M. Anglada, R. Sayós

Ab initio $^1A'$ ground potential energy surface and transition state theory kinetics study of the $O(^1D) + N_2O \rightarrow 2 NO, N_2 + O_2(a^1\Delta_g)$ reactions

Journal of Chemical Physics 115, 7015-7031 (2001)

M. González, M.P. Puyuelo, J. Hernando, R. Martínez, R. Sayós, P.A. Enríquez

Nascent $OH(X^2\Pi)$ product state distributions from the reaction of $O(^1D)$ with ethylene. A laser-induced fluorescence study

Chemical Physics Letters 346, 69-80 (2001)

M.J. Lakin, D. Troya, G. Lendvay, M. González, G.C. Schatz

A quasiclassical trajectory study of product energy and angular distributions for the $OH + D_2$ reaction

Journal of Chemical Physics 115, 5160-5169 (2001)

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M. González, R. Valero, R. Sayós

Ab initio ground potential energy surface ($^3A''$) for the $O(^3P) + N_2O$ reaction and kinetics study

Journal of Chemical Physics 115, 2540-2549 (2001)

M. González, I. Miquel, R. Sayós

Ab initio, variational transition state theory and quasiclassical trajectory study on the lowest $^2A'$ potential energy surface involved in the $N(^2D) + O_2(X^3\Sigma_g^-) \rightarrow O(^3P) + NO(X^2\Pi)$ atmospheric reaction

Journal of Chemical Physics 115, 2530-2539 (2001)

Troya, G. Lendvay, M. González, G.C. Schatz

A quasiclassical trajectory study of angular and internal state distributions in $H + H_2O$ and $H + D_2O$ at $E_T=1.4$ eV

Chemical Physics Letters 343, 420-428 (2001)

M. González, R. Valero, R. Sayós

Ab initio and DFT study of the ground $^3A'$ potential energy surface for the $O(^3P) + N_2O \rightarrow 2 NO$ reaction

Chemical Physics Letters 343, 119-129 (2001)

D. Troya, M.J. Lakin, G.C. Schatz, M. González

Variational transition state theory and quasiclassical trajectory studies of the $H_2 + OH \rightarrow H + H_2O$ reaction and some isotopic variants

Journal of Chemical Physics 115, 1828-1842 (2001)

R. Sayós, C. Oliva, M. González

The lowest doublet and quartet potential energy surfaces involved in the $N(^4S) + O_2$ reaction. I. *Ab initio* study of the C_s -symmetry ($^2A'$, $^4A'$) abstraction and insertion mechanisms

Journal of Chemical Physics 115, 1287-1297 (2001)

R. Sayós, J. Hernando, M.P. Puyuelo, P.A. Enríquez, M. González

Collision energy effects on the dynamics of the reaction $O(^3P) + CH_4(X^1A_1) \rightarrow OH(X^2\Pi) + CH_3(X^2A_2'')$

Chemical Physics Letters 341, 608-618 (2001)

H. Szichman, M. Gilibert, M. González, X. Giménez, A. Aguilar

A four dimensional quantum mechanical state-to-state study of the $H_2 + C_2H \rightarrow H + C_2H_2$ reaction

Journal of Chemical Physics 114, 9882-9893 (2001)

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D. Troya, M. González, G.C. Schatz

A quasiclassical trajectory study of reactivity and product energy disposal in $\text{H}+\text{H}_2\text{O}$, $\text{H}+\text{D}_2\text{O}$, and $\text{H}+\text{HOD}$
Journal of Chemical Physics 114, 8397-8413 (2001)

D. Troya, M. González, G. Wu, G.C. Schatz

A quasiclassical trajectory study of the $\text{Cl} + \text{HCN} \rightarrow \text{HCl} + \text{CN}$ reaction dynamics. Microscopic reaction mechanism of the $\text{H}(\text{Cl}) + \text{HCN} \rightarrow \text{H}_2(\text{HCl}) + \text{CN}$ reactions
Journal of Physical Chemistry A 105, 2285-2297 (2001)

M. González, I. Miquel, R. Sayós

VTST kinetics study of the $\text{N}(^2\text{D}) + \text{O}_2(\text{X}^3\Sigma_g^-) \rightarrow \text{NO}(\text{X}^2\Pi) + \text{O}(^3\text{P}, ^1\text{D})$ reactions based on CASSCF and CAPT2 ab initio calculations including excited potential energy surfaces
Chemical Physics Letters 335, 339-347 (2001)

M. González, R. Valero, R. Sayós

Ab initio and quasiclassical trajectory study of the $\text{N}(^2\text{D}) + \text{NO}(\text{X}^2\Pi) \rightarrow \text{O}(^1\text{D}) + \text{N}_2(\text{X}^1\Sigma_g^+)$ reaction on the lowest $^1\text{A}'$ potential energy surface
Journal of Chemical Physics 113, 10983-10998 (2000)

A. Aguilar, M. González, L.V. Poluyanov

Semiclassical approach to the non-adiabatic dynamics problem involving three electronic states in linear triatomic systems
Journal of Physics B 33, 4815-4820 (2000)

2000

M. González, J. Hernando, M.P. Puyuelo, R. Sayós

Theoretical study of the dynamics, stereodynamics and microscopic mechanism of the $\text{O}(^1\text{D}) + \text{CH}_4(\text{X}^1\text{A}_1) \rightarrow \text{OH}(\text{X}^2\Pi) + \text{CH}_3(\text{X}^2\text{A}_2'')$ reaction
Journal of Chemical Physics 113, 6748-6759 (2000)

R. Sayós, C. Oliva, M. González

A theoretical approach to the $\text{O}(^1\text{D}) + \text{H}_2\text{O}(\text{X}^1\text{A}_1)$ reaction: *Ab initio* potential energy surface and quasiclassical trajectory dynamics study
Journal of Chemical Physics 113, 6736-6747 (2000)

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D. Troya, I. Baños, M. González, G. Wu, M.A. ter Horst, G.C. Schatz

A quasiclassical trajectory study of the $\text{H} + \text{HCN} \rightarrow \text{H}_2 + \text{CN}$ reaction dynamics

Journal of Chemical Physics 113, 6253-6263 (2000)

H. Szichman, M. Gilibert, M. González, X. Giménez, A. Aguilar

Four-dimensional quantum mechanical treatment of penta-atomic systems: Case $\text{H}_2 + \text{C}_2\text{H} \rightarrow \text{H} + \text{C}_2\text{H}_2$; total reactive probabilities, cross-sections and rate constants

Journal of Chemical Physics 113, 176-183 (2000)

M. González, D. Troya, R. Sayós, J. Millán

A QCT study of the $\text{F} + \text{CH}_4 \rightarrow \text{HF} + \text{CH}_3$ reaction dynamics under thermal conditions

Lecture Notes in Chemistry 75, 303-308 (2000)

R. Sayós, C. Oliva, M. González

Quasiclassical trajectory study of the $\text{O}(^1\text{D}) + \text{H}_2\text{O} \rightarrow 2 \text{OH}$, $\text{H} + \text{HO}_2$ reactions

Lecture Notes in Chemistry 75, 279-285 (2000)

R. Sayós, R. Valero, J.M. Anglada, M. González

Theoretical investigation of the eight low-lying electronic states of the cis- and trans-nitric oxide dimers and its isomerization using multiconfigurational second-order perturbation theory (CASPT2)

Journal of Chemical Physics 112, 6608-6624 (2000)

R. Sayós, J. Hernando, R. Francia, M. González

Quasiclassical trajectory study of the $\text{H} + \text{ClF} \rightarrow \text{F} + \text{HCl}$, $\text{Cl} + \text{HF}$ and $\text{F} + \text{HCl} \rightarrow \text{Cl} + \text{HF}$ reactions and their deuterium isotope variants on a new ($^2\text{A}'$) *ab initio* potential energy surface

Physical Chemistry Chemical Physics 2, 523-533 (2000)

M. González, M.P. Puyuelo, J. Hernando, R. Sayós, P.A. Enríquez, J. Guayar, I. Baños

Influence of the collision energy on the $\text{O}(^1\text{D}) + \text{RH} \rightarrow \text{OH}(\text{X}^2\Sigma^-) + \text{R}$ ($\text{RH}=\text{CH}_4$, C_2H_6 , C_3H_8) reaction dynamics. A laser induced fluorescence and quasiclassical trajectory study

Journal of Physical Chemistry A 104, 521-529 (2000)

M. González, J. Hernando, I. Baños, R. Sayós

Ab initio ground potential energy surface and quasiclassical trajectory study of the $\text{O}(^1\text{D}) + \text{CH}_4(\text{X}^1\text{A}_1) \rightarrow \text{OH}(\text{X}^2\Pi) + \text{CH}_3(\text{X}^2\text{A}_2'')$ reaction dynamics

Journal of Chemical Physics 111, 8913-8924 (1999)

1999

M. González, J. Hernando, J. Millán, R. Sayós

Ab initio ground potential energy surface, VTST and QCT study of the $O(^3P) + CH_4(X^1A_1) \rightarrow OH(X^2\Sigma^-) + CH_3(X^2A_2'')$ reaction

Journal of Chemical Physics 110, 7326-7338 (1999)

R. Sayós, J. Hernando, J. Hijazo, M. González

An analytical potential energy surface of the $HCIF(^2A')$ system based on *ab initio* calculations. Variational transition state theory study of the $H + ClF \rightarrow F + HCl$, $Cl + HF$ and $F + HCl \rightarrow Cl + HF$ reactions and their deuterium isotope variants

Physical Chemistry Chemical Physics 1, 947-956 (1999)

M. Gilibert, X. Giménez, F. Huarte-Larrañaga, M. González, A. Aguilar, I. Last, M. Baer

Accurate 3D quantum dynamical study of the $Ne + H_2^+ \rightarrow NeH^+ + H$ reaction

Journal of Chemical Physics 110, 6278-6287 (1999)

M. González, D. Troya, M.P. Puyuelo, R. Sayós, P.A. Enríquez

The dynamics of the $O(^1D) + N_2O \rightarrow NO + NO$ reaction revisited: a QCT study on model potential energy surfaces

Chemical Physics Letters 300, 603-612 (1999)

1998

M. González, J. Hijazo, J.J. Novoa, R. Sayós

An analytical representation of the ground potential energy surface ($^2A'$) of the $H + Cl_2 \rightarrow HCl + Cl$ and $Cl + HCl \rightarrow HCl + Cl$ reactions, based on *ab initio* calculations

Journal of Chemical Physics 108, 3168-3177 (1998)

R. Sayós, J. Hijazo, M. Gilibert, M. González

Variational transition state calculation of the rate constants for the $N(^4S_u) + O_2(X^3\Sigma_g^-) \rightarrow NO(X^2\Pi) + O(^3P_g)$ reaction and its reverse between 300 and 5000 K

Chemical Physics Letters 284, 101-108 (1998)

1997

M. González, J. Hernando, R. Sayós, M.P. Puyuelo, P.A. Enríquez, J. Guayar, I. Baños

On the translational energy effect on the OH internal energy distribution arising from the reaction of $O(^1D)$ with alkanes (General Discussion)

Faraday Discussions 108, 453-457 (1997)

M. González, R. Sayós, P.A. Enríquez, D. Troya, M.P. Puyuelo

On the production mechanism of highly excited NO from the $O(^1D) + N_2O$ reaction (General Discussion)

Faraday Discussions 108, 449-453 (1997)

M. González, J.D. Sierra, R. Francia, R. Sayós

Quasiclassical trajectory study of molecular alignment effects on the dynamics of the reactions of Cl, Br and I with H_2

Journal of Physical Chemistry A 101, 7513-7521 (1997)

M. Gilibert, R.M. Blasco, M. González, X. Giménez, A. Aguilar, I. Last, M. Baer

Three dimensional quantum mechanical treatment of the reaction $Ne + H_2^+ \rightarrow NeH^+ + H$

Journal of Physical Chemistry A 101, 6821-6823 (1997)

I. Last, A. Aguilar, R. Sayós, M. González, M. Gilibert

Potential energy surface of the $O(^1D) + N_2O \rightarrow 2 NO$, $O_2 + N_2$ reactions

Journal of Physical Chemistry A 101, 1206-1215 (1997)

1996

M. González, J. Hijazo, J.J. Novoa, R. Sayós

An *ab initio* analytical potential energy surface for the $O(^3P) + CS(X^1\Sigma^+) \rightarrow CO(X^1\Sigma^+) + S(^3P)$ reaction useful for kinetic and dynamical studies

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