Grup de Cinética i Dinàmica de Reaccions Químiques UR – UB.

Llista de publicacions ordenades per anys de publicación. Actualitzada fins a finals juny l'any 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 $Ne + H_2^+(v_0 = 0\text{-}4, j_0 = 1) \rightarrow NeH^+ + H$ 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)

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P. Defazio, P. Gamallo, M. González, C. Petrongolo
Renner-Teller quantum dynamics of the NH(a1Δ) + H reactions on the NH_2 A^2A_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 N + NO $\rightarrow$ N_2 + O, NO + N atmospheric reactions
Journal of Chemical Physics 132, 144304-1/-9 (2010)

P. Defazio, P. Gamallo, M. González, S. Akpinar, B. Bussery-Honvault, P. Honvault, C. Petrongolo
Quantum dynamics of the C(^{1}D) + HD and C(^{1}D) + n-D_2 reactions on the $\tilde{a}^1$A' and b^1A" surfaces
Journal of Chemical Physics 132, 104306-1/-8 (2010)

2009

J.D. Sierra, R. Martínez, J. Hernando, M. González
The OH + D_2 $\rightarrow$ HOD + D angle-velocity distribution: Quasi-classical trajectory calculations on the YZCL2 and WSLFH potential energy surfaces and comparison with experiments at E_T = 0.28 eV
Physical Chemistry Chemical Physics 113, 11520-11527 (2009)

J. Mayneris-Perxachs, M. González
Time-dependent quantum dynamics study of the Ne + H_2^+(v=0-9) and D_2^+(v=0-12) proton transfer reactions at thermal collision energies
Journal of Physical Chemistry A 113, 4105-4109 (2009)

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P. Gamallo, P. Defazio, M. González, C. Petrongolo
Renner-Teller coupled-channel dynamics of the $N(^2D) + H_2$ reaction and the role of the NH_2 A^2A_1 electronic state
Journal of Chemical Physics 129, 244307-1/-5 (2008)

J. Mayneris, M. González, S. K. Gray
Real wavepacket code for ABC + D → 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) → 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) → 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 → 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)

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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)

P. Gamallo, R. Sayós, M. González, C. Petrongolo, P. Defazio
Quantum real wave-packet dynamics of the $N(^4S) + NO(X^2\Pi) \rightarrow N_2(X\ ^1\Sigma_g^+) + O(^3P)$ 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. Golfield, M. González, E. García, S.K. Gray
Theoretical study of the complex forming $CH + H_2 \rightarrow CH_2 + H$ 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 $O^+ + H_2(v=0, j=0) \rightarrow OH^+ + H$ ion-molecule reaction and comparison with quasiclassical trajectory calculations
Journal of Chemical Physics 124, 144301-1/-9 (2006)

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R. Martínez, J.D. Sierra, M. González
Cross sections of the $O^+ + H_2 \rightarrow OH^+ + H$ 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 LiH + H reactions
Journal of Chemical Physics 122, 214303-1/-9 (2005)

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J.D. Sierra, P.A. Enríquez, D. Troya, M. González
A QCT study of the cross-section, energy and angular distributions of the $OH + D_2 \rightarrow HOD + D$ 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 F + $CH_4 \rightarrow$ HF + CH_3 reaction

Journal of Chemical Physics 120, 5181-5191 (2004)

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 $1^3A"$ $N(^4S)$ + $NO(X^2\Pi) \rightarrow N_2(X^1\square_g^+)$ + $O(^3P)$ 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 $Cl + CH_4 \rightarrow HCl + CH_3$
Journal of Chemical Physics 117, 5730-5741 (2002)

P. Defazio, C. Petrongolo, C. Oliva, M. González, R. Sayós
Quantum dynamics of the $N(^4S) + O_2$ reaction on the X^2A' and a^4A' 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 $H + CO_2 \rightarrow OH + CO$ reaction
Journal of Physical Chemistry B 106, 8148-8160 (2002)

M. González, I. Miquel, R. Sayós
Ab initio, VTST, and QCT study of the $3^2A'$ potential energy surface implied in the $N(^2D) + O_2(X^3\Sigma_g^-) \rightarrow O(^3P) + NO(X^2\Pi)$ 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 $N(^4S) + O_2$ 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 ($^2A'$, $^4A'$) surfaces and theoretical rate constants for the $N(^4S) + O_2$ reaction
Journal of Chemical Physics 117, 670-679 (2002)

M. González, R. Valero, R. Sayós
Ab initio and kinetics study of the ground ^{1}A" potential energy surface of the O(^{1}D) + N_2O →2 NO, N_2 + O_2(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 O(^{1}D) + CH_4(X^1A_1) → OH($X^2\Pi$) + CH_3(X^2A_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(^{2}D) + O_2($X^3\Sigma_g^-$) → O(^{3}P) + 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(^{1}D) + 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 → 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(^{1}D) 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 ^{1}A' ground potential energy surface and transition state theory kinetics study of the O(^{1}D) + N_2O → 2 NO, N_2 + O_2($a^1\Delta_g$) reactions
Journal of Chemical Physics 115, 7015-7031 (2001)

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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(^{1}D) 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)

M. González, R. Valero, R. Sayós
Ab initio ground potential energy surface (^{3}A") for the O(^{3}P) + 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 ^{2}A' potential energy surface involved in the N(^{2}D) + $O_2(X^3\Sigma_g^-) \rightarrow$ O(^{3}P) + 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 ^{3}A' potential energy surface for the O(^{3}P) + $N_2O \rightarrow$ 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(^{4}S) + O_2 reaction. I. *Ab initio* study of the C_s-symmetry (^{2}A', ^{4}A') abstraction and insertion mechanisms
Journal of Chemical Physics 115, 1287-1297 (2001)

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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)

D. Troya, M. González, G.C. Schatz
A quasiclassical trajectory study of reactivity and product energy disposal in $H+H_2O$, $H+D_2O$, and H+HOD
Journal of Chemical Physics 114, 8397-8413 (2001)

D. Troya, M. González, G. Wu, G.C. Schatz
A quasiclassical trajectory study of the Cl + HCN → HCl + CN reaction dynamics. Microscopic reaction mechanism of the H(Cl) + HCN → H_2(HCl) + CN reactions
Journal of Physical Chemistry A 105, 2285-2297 (2001)

M. González, I. Miquel, R. Sayós
VTST kinetics study of the $N(^2D) + O_2(X^3\Sigma_g^-) \rightarrow NO(X^2\Pi) + O(^3P,^1D)$ 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 $N(^2D) + NO(X^2\Pi) \rightarrow O(^1D) + N_2(X^1\Sigma_g^+)$ reaction on the lowest $^1A'$ 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)

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M. González, J. Hernando, M.P. Puyuelo, R. Sayós
Theoretical study of the dynamics, stereodynamics and microscopic mechanism of the $O(^1D) + CH_4(X^1A_1) \rightarrow OH(X^2\Pi) + CH_3(X^2A_2")$ reaction
Journal of Chemical Physics 113, 6748-6759 (2000)

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R. Sayós, C. Oliva, M. González

A theoretical approach to the $O(^1D)$ + $H_2O(X^1A_1)$ reaction: *Ab initio* potential energy surface and quasiclassical trajectory dynamics study

Journal of Chemical Physics 113, 6736-6747 (2000)

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

A quasiclassical trajectory study of the H + HCN $\rightarrow$ H_2 + 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 H_2 + C_2H $\rightarrow$ H + C_2H_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 F + CH_4 $\rightarrow$ HF + 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 $O(^1D)$ + H_2O $\rightarrow$ 2 OH, H + 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 muticonfigurational 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 H + ClF $\rightarrow$ F + HCl, Cl + HF and F + HCl $\rightarrow$ Cl + HF reactions and their deuterium isotope variants on a new (^{2}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 $O(^1D)$ + RH $\rightarrow$ $OH(X^2\square)$ + R (RH=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 $O(^1D) + CH_4(X^1A_1) \rightarrow OH(X^2\Pi) + CH_3(X^2A_2")$ reaction dynamics

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

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

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

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

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

An analytical potential energy surface of the $HClF(^2A')$ 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)

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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)

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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

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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)

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On the production mechanism of highly excited NO from the $O(^1D) + N_2O$ reaction (General Discussion)
Faraday Discussions 108, 449-453 (1997)

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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)

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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
Journal of Chemical Physics 105, 10999-11006 (1996)

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Chemical Physics 209, 355-365 (1996)

M. Gilibert, M. González, R. Sayós, A. Aguilar, X. Giménez, J. Hijazo
Reactive cross sections involving atomic nitrogen and ground and vibrationally excited molecular oxygen and nitric oxide
Molecular Physics and Hypersonic Flows, M. Capitelli (Ed.)
Kluwer Academic Publishers, Dordrecht, 53-84 (1996)

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M. González, M. Gilibert, A. Aguilar, R. Sayós
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Chemical Physics 200, 289-308 (1995)

A. Aguilar, M. Gilibert, X. Giménez, M. González, R. Sayós
Dynamics of the $N(^4S_u)$ + $NO(X^2\Pi)$ → $N_2(X^1\Sigma_g^+)$ + $O(^3P_g)$ atmospheric reaction on the $^3A''$ ground potential energy surface. III. Quantum dynamical study and comparison with quasiclassical and experimental results
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J. Hijazo, M. González, R. Sayós, J.J. Novoa
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