

**Publications of Joel M. Bowman
Prior to 2006**

202. Quantum inelastic scattering study of isotope effects in ozone stabilization dynamics, T. Xie, J. M. Bowman, Chem. Phys. Lett. **412**, 131-134 (2005).
203. Quantum studies of the vibrations in H_3O_2^- and D_3O_2^- , A. B. McCoy, X. Huang, S. Carter, and J. M. Bowman, J. Chem. Phys. **123**, 064317 (2005).
204. The vibrational predissociation spectra of the $\text{H}_5\text{O}_2^+ \cdot \text{RG}_n$ ($\text{RG} = \text{Ar}, \text{Ne}$) clusters: Correlation of the solvent perturbations in the free OH and shared proton transitions of the Zundel ion, N. I. Hammer, E. G. Diken, J. R. Roscioli, E. M. Myshakin, K. D. Jordan, A. B. McCoy, X. Huang, S. Carter, J. M. Bowman, and M. A. Johnson, J. Chem. Phys. **122**, 244301 (2005).
205. *Ab initio* Global Potential Energy Surface for $\text{H}_5^+ \rightarrow \text{H}_3^+ + \text{H}_2$, Z. Xie, B. J. Braams, and J. M. Bowman J. Chem. Phys. **122**, 224307 (2005).
206. Quasiclassical trajectory study of formaldehyde: $\text{H}_2\text{CO} \rightarrow \text{H}_2 + \text{CO}$, $\text{H} + \text{HCO}$, X. Zhang, J. L. Rheinecker, and J. M. Bowman, J. Chem. Phys. **122**, 114313 (2005).
207. Full-dimensional vibrational calculations for H_5O_2^+ using an *ab initio* potential energy surface, A. B. McCoy, X. Huang, S. Carter, M. Landeweer, and J. M. Bowman, J. Chem. Phys. **122**, 061101 (2005).
208. *Ab initio* potential energy and dipole moment surfaces for H_5O_2^+ , X. Huang, B. J. Braams, and J. M. Bowman, J. Chem. Phys. **122**, 044308 (2005).
209. Progress in the quantum description of vibrational motion of polyatomic molecules, J. M. Bowman, S. Carter, and N. C. Handy, in Theory and Applications of Computational Chemistry: The First 40 Years, eds. C. Dykstra, G. Frenking, K S. Kim and G E. Scuseria (Elsevier, Amsterdam, 2005), pp. 251-267.
210. The roaming atom: Straying from the reaction path in formaldehyde decomposition, D. Townsend, S. A. Lahankar, S. K. Lee, S. D. Chambreau, A. G. Suits, X. Zhang, J. Rheinecker, L. B. Harding and J. M. Bowman, Science **306**, 1158-1161 (2004).
211. Argon predissociation spectroscopy of the $\text{OH}^- \cdot \text{H}_2\text{O}$ and $\text{Cl}^- \cdot \text{H}_2\text{O}$ complexes in the 1000 – 1900 cm^{-1} region: Intramolecular bending transitions and the search for the shared proton fundamental in the hydroxide monohydrate, E. G. Diken, J. M. Headrick, J. R. Roscioli, J. C. Bopp, M. A. Johnson, A. B. McCoy, X. Huang, S. Carter, and J. M. Bowman, J. Phys. Chem. **A109** 571-575 (2005)

212. Quasiclassical trajectory studies of the dynamics of H_2CO on a global *ab initio*-based potential energy surface, J. L. Rheinecker, X. Zhang, and J. M. Bowman, *Mol. Phys.* **103**, 1067-1074 (2005).
213. The roaming atom: Straying from the reaction path in formaldehyde decomposition, D. Townsend, S. A. Lahankar, S. K. Lee, S. D. Chambreau, A. G. Suits, X. Zhang, J. Rheinecker, L. B. Harding and J. M. Bowman, *Science* **306**, 1158-1161 (2004).
214. Calculation of converged rovibrational energies and partition function for methane using vibrational-rotational configuration interaction, A. Chakraborty, D. G. Truhlar, J. M. Bowman, and S. Carter, *J. Chem. Phys.* **121**, 2071-2084 (2004).
215. Quantum and quasi-classical studies of the $\text{O}(^3\text{P}) + \text{HCl} \rightarrow \text{OH} + \text{Cl}(^2\text{P})$ reaction using benchmark potential surfaces, T. Xie, J. M. Bowman, J. W. Duff and M. Braunstein, and B. Ramachandran, *J. Chem. Phys.* **122**, 014301 (2005).
216. Construction of a global potential energy surface from novel *ab initio* molecular dynamics for the $\text{O}(^3\text{P}) + \text{C}_3\text{H}_3$ reaction, S. C. Park, B. J. Braams, and J. M. Bowman, *J. Theor. Comput. Chem.* **4**, 163-173 (2005).
217. Enhancement of tunneling due to resonances in pre-barrier wells in chemical reactions, J. M. Bowman, *Chem. Phys.* **308**, 255-257 (2005).
218. Normal mode analysis using the driven molecular dynamics method. II. An application to biological macromolecules, M. Kaledin, A. Brown, A. Kaledin, and J. M. Bowman, *J. Chem. Phys.* **121**, 5646-5653 (2004).
219. *Ab initio* Diffusion Monte Carlo calculations of the quantum behavior of CH_5^+ in full dimensionality, A. B. McCoy, B. J. Braams, A. Brown, X. Huang, Z. Jin and J. M. Bowman, *J. Phys. Chem. A* **108**, 4991-4994 (2004).
220. Experimental and theoretical study of the infrared spectra of BrHI^- and BrDI^- , M. J. Nee, A. D. Osterwalder, D. M. Neumark, C. Kaposta, C. C. Uhalte, T. Xie, A. L. Kaledin, J. M. Bowman, S. Carter, and K. R. Asmis, *J. Chem. Phys.* **121**, 75297268 (2004).
221. A global *ab initio* potential energy surface for formaldehyde, X.-B. Zhang, S.-L. Zou, L. B. Harding, and J. M. Bowman, *J. Phys. Chem. A* **108**, 8980-8986 (2004).
222. Quantum calculations of vibrational energies of H_3O_2^- on an *ab initio* potential, X. Huang, B. J. Braams, S. Carter, J. M. Bowman, *J. Am. Chem. Soc.* **126**, 5042-5043 (2004).
223. A reduced dimensionality quasi-classical and quantum study of the proton transfer reaction $\text{H}_3\text{O}^+ + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O} + \text{H}_3\text{O}^+$, J. Rheinecker, T. Xie, and J. M. Bowman, *J. Chem. Phys.* **120**, 7018-7023 (2004).

224. Comparison of classical, new corrected-classical, and semiclassical IR spectra of non-rotating H₂O with quantum calculations, A. L. Kaledin, X. Huang and J. M. Bowman, Chem. Phys. Lett. **384**, 80-85 (2004).
225. Quantum and classical studies of vibrational motion of CH₅⁺ on a global potential energy surface obtained from a novel *ab initio* direct dynamics approach, A. Brown, A. B. McCoy, B. J. Braams, Z. Jin, and J. M. Bowman, J. Chem. Phys., **121**, 4105-4116 (2004).
226. 'Morphing' of *ab initio*-based interaction potentials to spectroscopic accuracy: Application to Cl⁻(H₂O), J. M. Bowman and S. S. Xantheas, Pure Appl. Chem., **76**, 29-35 (2004).
227. The Internal Coordinate Path Hamiltonian; application to methanol and malonaldehyde, D. P. Tew, N. C. Handy, S. Carter, S. Irle, and J. M. Bowman, Mol. Phys. **101**, 3513-3525 (2003).
228. A theoretical study of vibrational mode coupling in H₅O₂⁺, J. Dai, Z. Bacic, X. Huang, S. Carter, and J. M. Bowman, J. Chem. Phys. **119**, 6571-6580 (2003).
229. Quantum calculations of the rate constant for the O(³P) + HCl reaction on new *ab initio* ³A" and ³A' surfaces, T. Xie, J. M. Bowman, K. A. Peterson, and B. Ramuchandran, J. Chem. Phys. **119**, 9601-9608 (2003).
230. Classical and quasiclassical spectral analysis of CH₅⁺ using an *ab initio* potential energy surface, A. Brown, B. J. Braams, K. M. Christoffel, Z. Jin, and J. M. Bowman, J. Chem. Phys. **119**, 8790-8793 (2003).
231. A scaled *ab initio* potential energy surface for acetylene and vinylidene, D. Xu, H. Guo, S.-L. Zou, and J. M. Bowman, Chem. Phys. Lett. **377**, 582-588 (2003).
232. MULTIMODE: A code to calculate rovibrational energies of polyatomic molecules, J. M. Bowman, S. Carter, and X. Huang, Int. Rev. Phys. Chem. **22**, 533-549 (2003).
233. Normal-mode analysis without the Hessian: A driven molecular dynamics approach, J. M. Bowman, X.-B. Zhang and A. Brown, J. Chem. Phys. **119**, 646-650 (2003).
234. Full dimensional quantum calculations of the vibrational energies of H₅O₂⁺, X. Huang, H. M. Cho, S. Carter, L. Ojamäe, J. M. Bowman, and S. J. Singer, J. Phys. Chem. A **107**, 7142-7151 (2003).
235. Full-dimensionality quantum calculations of acetylene ↔ vinylidene isomerization, S.-L. Zou, J. M. Bowman, and A. Brown, J. Chem. Phys. **118**, 10012-10023 (2003).
236. *Ab initio* potential energy surface and rovibrational energies of H₃O⁺ and its isotopomers, X. Huang, S. Carter and J. M. Bowman, J. Chem. Phys. **118**, 5431-5441 (2003).

237. A new *ab initio* potential energy surface describing acetylene/vinylidene isomerization, J. M. Bowman and S.-L. Zou, Chem. Phys. Lett. **368**, 421-424 (2003).
238. Radiative relaxation and isomeric branching of highly excited H/C/N: The importance of delocalized vibrational states T. Barger, A. M. Wodtke, and J. M. Bowman, Ap. J., **587**, 841-846 (2003).
239. "Atomic and Molecular Collisions," R. E. Johnson and J. M. Bowman, in *Encyclopedia of Physical Science and Technology (Third Edition)*, edited by R. A. Meyers (Academic Press, New York, 2003), Vol. 1, pp. 721-744.
240. On using potential, gradient, and Hessian data in least squares fits of potentials: Application and tests for H₂O, T. Xie and J. M. Bowman, J. Chem. Phys. **117**, 10487-10492 (2002).
241. Full dimensionality quantum calculations of acetylene/vinylidene isomerization, S.-L. Zou and J. M. Bowman, J. Chem. Phys. **117**, 5507-5510 (2002).
242. *Ab initio* potential energy surface and vibrational energies of H₃O⁺ and its isotopomers, X. Huang, S. Carter and J. M. Bowman, J. Phys. Chem. B, **106**, 81828188 (2002).
243. Overview of reduced dimensionality quantum approaches to reactive scattering, J. M. Bowman, Theor. Chem. Acc. **108**, 125-133 (2002).
244. Resonances in the O(³P)+HCl reaction due to Van der Waals minima, T. Xie, D. Wang, J. M. Bowman, and D. E. Manolopoulos, J. Chem. Phys. **116**, 7461-7467 (2002).
245. Reduced dimensionality quantum calculations of acetylene ↔ vinylidene isomerization, S.-L. Zou and Joel M. Bowman, J. Chem. Phys. **116**, 6667-6673 (2002).
246. A quasiclassical trajectory study of O(¹D)+HCl reactive scattering on an improved *ab initio* surface, K. M. Christoffel and J. M. Bowman, J. Chem. Phys. **116**, 4842-4846 (2002).
247. Full dimensional calculations of vibrational energies of H₃O⁺ and D₃O⁺, J. M. Bowman, X. Huang, and S. Carter, Spec. Acta A **58**, 839-848 (2002).
248. The vibrational levels of ammonia, C. Leonard, N. C. Handy, S. Carter, and J. M. Bowman, Spec. Acta A **58**, 825-838 (2002).
249. Characterization of the sulfur fluoride radical in the ground electronic state, I. M. B. Nielsen, S.-L. Zou, J. M. Bowman, and C. L. Janssen, Chem. Phys. Lett. **352**, 26-32 (2002).
250. The challenge of high resolution dynamics: Rotationally mediated unimolecular dissociation of HOCl, J. M. Bowman, S. Skokov, S.-L. Zou, and K. A. Peterson, in *Symposium Series No. 828/Low-Lying*

Potential Energy Surfaces, edited by M. Hoffman and K. G. Dyall (ACS, Washington, DC, 2002), 346-360.

251. The unimolecular dissociation of the OH stretching states of HOCl: Comparison with experimental data, J. Weiss, J. Hauschildt, R. Schinke, O. Haan, S. Skokov, J. M. Bowman, V. A. Mandelshtam, and K. A. Peterson, *J. Chem. Phys.* **115**, 8880-8887 (2001).
252. A reduced dimensionality, six-degree-of-freedom, quantum calculation of the $\text{H} + \text{CH}_4 \rightarrow \text{H}_2 + \text{CH}_3$ reaction, D. Wang and J. M. Bowman, *J. Chem. Phys.* **115**, 2055-2061 (2001).
253. On using low-order Hermite interpolation in "direct dynamics" calculations of vibrational energies using the code "MULTIMODE", S. Carter, J. M. Bowman, and B. J. Braams, *Chem. Phys. Lett.* **342**, 636-642 (2001).
254. The importance of an accurate CH_4 vibrational partition function in full dimensionality calculations of the $\text{H} + \text{CH}_4 \rightarrow \text{H}_2 + \text{CH}_3$ reaction, J. M. Bowman, D. Y. Wang, X. Huang, F. Huarte-Larranaga, and U. Manthe, *J. Chem. Phys.* **114**, 9683-9684 (2001).
255. Dipole moments of highly vibrationally excited HCN: Theoretical prediction of an experimental diagnostic for delocalized states, J. M. Bowman, S. Irle, K. Morokuma, and A. Wodtke, *J. Chem. Phys.* **114**, 7923-7934 (2001).
256. State-to-state reactive scattering via real L^2 wave packet propagation for reduced dimensionality AB + CD reactions, S. Skokov and J. M. Bowman, *J. Phys. Chem. A* **105**, 2502-2508 (2001).
257. Tribute to Aron Kuppermann, J. M. Bowman, J. A. Kaye, G. C. Schatz, and D. G. Truhlar, *J. Phys. Chem. A* **105**, 2127-2128 (2001).
258. Adiabatic rotation, centrifugal sudden, and exact calculations of rotationally mediated Fermi resonances in HOCl, S. L. Zou, S. Skokov, and J. M. Bowman, *J. Phys. Chem. A* **105**, 2423-2426 (2001).
259. A local interpolation method for direct classical dynamics calculations, K. M. Christoffel, J. M. Bowman, and B. J. Braams, *J. Chem. Phys.* **115**, 11021-11024 (2001).
260. Vibrational spectrum of the formic acid dimer in the OH stretch region. A model 3D study, M. V. Vener, O. Kuhn, and J. M. Bowman, *Chem. Phys. Lett.* **349**, 562-570 (2001).
261. *Ab initio* calculation of resonance energies and widths of HOCl($7\nu_{\text{OH}}$) and ($8\nu_{\text{OH}}$) and comparison with experiment, S. L. Zou, S. Skokov, and J. M. Bowman, *Chem. Phys. Lett.* **339**, 290-294 (2001).
262. Thermal and state-selected rate coefficients for the $\text{O}(^3\text{P}) + \text{HCl}$ reaction and new calculations of the barrier height and width, S. Skokov, S. L. Zou, J. M. Bowman, T. C. Allison, D. G. Truhlar, Y. J. Lin, B. Ramachandran, B. C. Garrett, and B. J. Lynch, *J. Phys. Chem. A* **105**, 2298-2307 (2001).

263. Direct *ab initio* variational calculation of vibrational energies of the $\text{H}_2\text{O}\cdots\text{Cl}^-$ complex and resolution of experimental differences, Stephan Irle and Joel M. Bowman, J. Chem. Phys. **113**, 8401-8403 (2000).
264. Vibrational dynamics up to the dissociation threshold: A case study of two-dimensional HOCl, M. Joyeaux, D. Sugny, M. Lombardi, R. Jost, R. Schinke, S. Skokov, and J. M. Bowman, J. Chem. Phys. **113**, 9610-9621 (2000).
265. Theoretical study of the photodetachment spectroscopy of the IBr and IBr⁻ anions, A. Kaledin, S. Skokov, J. M. Bowman, and K. Morokuma, J. Chem. Phys. **113**, 9479-9487 (2000).
266. Quantum calculations of the effect of bend excitation in methane on the HCl rotational distribution in the reaction $\text{CH}_4 + \text{Cl} \rightarrow \text{CH}_3 + \text{HCl}$, S. Skokov and J. M. Bowman, J. Chem. Phys. **113**, 4495-4497 (2000).
267. Beyond Platonic Molecules (An Invited "Perspective") J. M. Bowman, Science **290**, 724-725 (2000).
268. Quantum scattering calculations of the $\text{O}(^1\text{D}) + \text{HCl}$ reaction using a new *ab initio* potential and extensions of J-shifting, Martina Bittererova, Joel M. Bowman, and Kirk Peterson, J. Chem. Phys. **113**, 6186-6196 (2000).
269. A wavepacket calculation of the effect of reactant rotation and alignment on product branching in the $\text{O}(^1\text{D}) + \text{HCl} \rightarrow \text{ClO} + \text{H}$, $\text{OH} + \text{Cl}$ reactions, Martina Bittererova and Joel M. Bowman, J. Chem. Phys. **113**, 1-3 (2000).
270. A reduced dimensionality quantum calculation of the reaction of H_2 with diamond (111) surface, Sergei Skokov and Joel M. Bowman, J. Chem. Phys. **113**, 779-788 (2000).
271. A comparative study of quantum dynamics and rate constant for the $\text{O}(^3\text{P}) + \text{HCl}$ reaction described by two potential surfaces, S. Skokov, T. Tsuchida, S. Nambu, J. M. Bowman, and S. Gray, J. Chem. Phys. **113**, 227-236 (2000).
272. Quantum scattering calculations of energy transfer and isomerization of HCN/HNC in collisions with Ar, Kurt M. Christoffel and Joel M. Bowman, J. Chem. Phys. **112**, 4496-4505 (2000).
273. Wavepacket propagation for reactive scattering using real L^2 eigenfunctions with damping, S. Skokov and J.M. Bowman, PCCP, **2**, 495-500 (2000).
274. Approximate time independent methods for polyatomic reactions, J. M. Bowman, in Reaction and Molecular Dynamics (Proceedings of the European School on Computational Chemistry, Perugia, Italy, July (1999)) Laganà, A., Riganelli, A., (Eds.), (Springer Berlin Heidelberg, 2000), Vol. 75, pp. 101-114
275. Variational calculations of rotational-vibrational energies of CH_4 and isotopomers using an adjusted *ab initio* potential, S. Carter and J. M. Bowman, J. Phys. Chem. A **104**, 2355-2361 (2000)

276. Perturbative inversion of the HOCl potential energy surface via singular value decomposition, S. Skokov, K. Peterson, and J. M. Bowman, Chem. Phys. Lett **312**, 494-502 (1999).
277. Quantum and quasiclassical reactive scattering of O(¹D)+HCl using an *ab initio* potential, Kurt Christoffel, a Yohan Kim, a Sergei Skokov, Joel M. Bowman and Stephen Gray, Chem. Phys. Lett. **315**, 275-281 (1999).
278. Theoretical Studies of Rotation Induced Fermi Resonances in HOCl, R. Chen, H. Guo, S. Skokov, and J. M. Bowman, J. Chem. Phys. **111**, 7290-7297 (1999).
279. A theoretical study of the vibrational energy spectrum of the HOCl/HClO system on an accurate *ab initio* potential energy surface, K. A. Peterson, S. Skokov, and J. M. Bowman, J. Chem. Phys. **111**, 7446-7456 (1999).
280. Complex L² calculation of the variation of resonance widths of HOCl with total angular momentum, Sergei Skokov and Joel M. Bowman, J. Chem. Phys. **111**, 4933-4941 (1999).
281. Vibrational Analysis of HOCl up to 98% of the dissociation energy with a Fermi Resonance Hamiltonian, Remy Jost, Marc Joyeaux, Sergei Skokov, and Joel M. Bowman, J. Chem. Phys. **111**, 6807-6820 (1999)
282. Variation of the resonance width of HOCl(6v_{OH}) with total angular momentum: Comparison between *ab initio* theory and experiment, Sergei Skokov and Joel M. Bowman, J. Chem. Phys. **110**, 9789-9792 (1999).
283. The spin-forbidden reaction CH(²Π)+N₂ → HCN+N(⁴S) revisited. II. Non-adiabatic transition state theory and application. Qiang Cui, Keiji Morokuma, Joel M. Bowman, and Stephen J. Klippenstein, J. Chem. Phys **110**, 9469-9482 (1999).
284. Potential energy surface and vibrational eigenstates of the H₂-CN(X²Σ⁺) van der Waals complex, Alexey L. Kaledin, Michael C. Heaven, and Joel M. Bowman, J. Chem. Phys. **110**, 10380-10392 (1999).
285. Variational calculations of rovibrational energies of CH₄ and isotopomers in full dimensionality using an *ab initio* potential, Stuart Carter, Heather M. Shnider, and Joel M. Bowman, J. Chem. Phys. **110**, 8417-8423 (1999).
286. RRKM theory beyond the separable harmonic approximation: The HCO₂ → H+CO₂ unimolecular dissociation, Kurt Christoffel and Joel M. Bowman, J. Phys. Chem. A **103**, 3020-3030 (1999).
287. Calculation of resonance states of non-rotating HOCl using an accurate *ab initio* potential, Sergei Skokov, Joel Bowman, and Vladimir Mandelshtam, Physical Chemistry Chemical Physics, **1**, 1279-1282 (1999).

288. Non-separable transition state theory for non zero total angular momentum: Implications for J shifting and application to the OH+H₂ reaction, Joel M. Bowman and Heather Shnider, J. Chem. Phys. **110**, 4428-4434 (1999).
289. Calculations of low-lying vibrational states of cis- and trans-HOCO, Joel M. Bowman, Kurt Christoffel, and Gabe Weinberg, J. Mol. Struct. (Theochem) **461-462**, 71-77 (1999).
290. Classical and quantum mechanical studies of the CO vibrations in CO/Cu(100), S. C. Park, W. K. Park and J. M. Bowman, Surf. Sci. **427-28**, 343-348 (1999).
291. Energetics and dynamics of Ar-water photodissociation, in Adv. Molec Vib and Coll. Dynamics: Molecular Clusters, Vol III, eds. J. M. Bowman and Z. Bacic, (JAI, Stamford CT, 1998), pp. 61-89.
292. Accurate variational calculations and analysis of the HOCl vibrational energy spectrum, Sergei Skokov, Jianxin Qi, Joel M. Bowman, Chao-Yie Yang, Stephen K. Gray, Kirk A. Peterson, and Vladimir A. Mandelshtam, J. Chem. Phys. **109**, 10273-10283 (1998).
293. Extensions and tests of 'multimode': A code to obtain accurate vibration/rotation energies of many-mode molecules, Stuart Carter, Joel M. Bowman and Nicholas Handy, Theor. Chem. Acc. **100**, 191-198 (1998).
294. An accurate *ab initio* HOCl potential energy surface, vibrational and rotational calculations, and comparison with experiment, S. Skokov, K. A. Peterson, and J. M. Bowman, J. Chem. Phys. **109**, 2662-2671 (1998).
295. Vibrational spectrum of (CO)₂ on Cu(100): Quantum calculations with 18 coupled modes, Fedor Dzegilenko, Joel M. Bowman and Stuart Carter, J. Chem. Phys. **109**, 7506-7510 (1998).
296. Quantum calculations of inelastic and dissociative scattering of HCO by Ar J. Qi and J. M. Bowman, J. Chem. Phys. **109**, 1734-1742 (1998).
297. Resonances: Bridge between spectroscopy and dynamics, invited Feature Article, J. Phys. Chem. **102**, 3006-3017 (1998).
298. The adiabatic rotation approximation for rovibrational energies of many-mode systems: Description and tests of the method, Stuart Carter and Joel M. Bowman, J. Chem. Phys. **108**, 4397-4404 (1998).
299. "Spectator" modes in resonance-driven reactions: Three-dimensional quantum calculations of HOCO resonances, F. N. Dzegilenko and J. M. Bowman, J. Chem. Phys. **108**, 511-518 (1998).
300. Generalized coordinate-scaling approach for optimization of potentials, J. M. Bowman and J. Qi, in *Fashioning a Model: Optimization Methods in Chemical Physics*, edited by A. Ernesti, J. M. Hutson, and N. J. Wright (CCP6, Daresbury, 1998), chapter 5.

301. Vibrational Self-Consistent Field Method for Many-Mode Systems: A New approach and application to the vibrations of CO adsorbed on Cu(100) S. Carter, S. J. Culik and J. M. Bowman, J. Chem. Phys. **107**, 10458-10469 (1997).
302. Approximations based on the adiabatic treatment of rotation for resonances, Jianxin Qi and Joel M. Bowman, J. Chem. Phys. **107**, 9960-9965 (1997).
303. A Test of *J*-Shifting for H+CO Recombination, J. Qi and J. M. Bowman, Chem. Phys. Lett. **276**, 371-374 (1997).
304. Two novel applications of Shepard-type interpolation for polyatomic systems: Reduced dimensionality HOCO and full dimensionality Ar-HCO, Fedor N. Dzegilenko, Jianxin Qi, and Joel M. Bowman, Int. J. Quantum Chem., Quantum Chem. Symp. No. 37, **65**, 965-973 (1997).
305. Inverse perturbation via singular value decomposition: Application to correction of potential surface for HCN, Qian Wu, John Z.H. Zhang, and Joel M. Bowman, J. Chem. Phys. **107**, 3602-3610 (1997).
306. A new perspective on isomerization dynamics illustrated by HCN→HNC, Bela Gazdy and Joel M. Bowman, J. Phys. Chem. A **101**, 6384-6388 (1997).
307. *Ab initio* Calculations of the Interaction Potentials of Ar-HCN and Ar-HCO, J. Qi, M. Dyksterhouse, and J. M. Bowman, ACS Symp Series 678 Highly Excited Molecules, eds. A. Mullin and G. C. Schatz (ACS, Washington D.C., 1997), pp. 150-172
308. *Ab initio* calculations of force fields for H₂CN and ClHCN and vibrational energies of H₂CN, Stuart Carter, Joel M. Bowman, and Lawrence B. Harding, Spectrochim. Acta **A53**, 1179-1188 (1997).
309. Non-Condon effects in photodissociation of ICN($\tilde{A} \leftarrow \tilde{X}$): Coupled-channel scattering calculations, Fedor N. Dzegilenko, Joel M. Bowman, and Y. Amatatsu, Chem. Phys. Lett. **264**, 24-30 (1997).
310. Complex L^2 calculations of resonances in HOCO, Joel M. Bowman and A. Metropoulos, J. Chem. Soc., Faraday Trans., **93**, 815-818 (1997).
311. The effect of rotation on resonances: Application to HCO, Jianxin Qi and Joel M. Bowman, J. Chem. Phys. **105**, 9884-9889 (1996)
312. Quantum calculation of the recombination rate constant of H+CO → HCO Jianxin Qi and Joel M. Bowman, J. Phys. Chem. **100**, 15165-15170 (1996).
313. Recovering a full dimensional quantum rate constant from a reduced dimensionality calculation: Application to the OH+CO→H+CO₂ reaction, Fedor N. Dzegilenko and Joel M. Bowman, J. Chem. Phys. **105**, 2280-2286 (1996).

314. Quasiclassical trajectory calculations of photodissociation of Ar-H₂O($\tilde{X}$ - $\tilde{A}$) and H₂O($\tilde{X}$ - $\tilde{A}$), Kurt M. Christoffel and Joel M. Bowman, J. Chem. Phys. **104**, 8348-8356 (1996).
315. Resonances in the cumulative reaction probability for a model electronically non-adiabatic reaction, Jianxin Qi and Joel M. Bowman, J. Chem. Phys. **104**, 7545-7553 (1996).
316. Quantum mechanical calculation of the CO vibrations in CO/Cu(100), Seung C. Park, Joel M. Bowman, and Daniel A. Jelski, J. Chem. Phys. **104**, 2457-2460 (1996)
317. Quantum calculations of inelastic scattering of HCN and HNC by Ar, J. M. Bowman and A. Padmavathi, Mol. Phys. **88**, 21-32 (1996).
318. A new vibrational self-consistent field program for large molecules, Daniel A. Jelski, Randall H. Haley, and Joel M. Bowman, J. Comp. Chem. **17**, 1654-1652 (1996).
319. Quantum scattering calculations of energy transfer and dissociation of HCO in collisions with Ar, B. Pan and J. M. Bowman, J. Chem. Phys. **103**, 9661-9668 (1995).
320. Ab initio characterization of the low-lying vibrations of HCO (DCO) in the $\tilde{B}^2A'$ State, J. Qi, J. M. Bowman, and R. Maana, J. Chem. Phys. **103**, 7664-7672 (1995).
321. Quantum scattering calculations for vibrational and rotational excitation of CO by hot hydrogen atoms, S. Green, B. Pan, and J. M. Bowman, J. Chem. Phys. **102**, 8800-8806 (1995).
322. An *ab initio* study of the ground and first excited state of HCN $\leftrightarrow$ HNC isomerization and a calculation of the HNC A $\rightarrow$ X fluorescence spectrum, B. Gazdy, D. G. Musaev, J. M. Bowman, and K. Morokuma, Chem. Phys. Lett. **237**, 27-32 (1995).
323. Adjusted double many-body expansion potential energy surface for HO₂ based on rigorous vibrational calculations, A.J.C. Varandas, J. M. Bowman, and B. Gazdy, Chem. Phys. Lett. **233**, 405-410 (1995).
324. Complex L^2 calculations of bound states and resonances of HCO and DCO, D. S. Wang and J. M. Bowman, Chem. Phys. Lett. **235**, 277-285 (1995).
325. Theoretical studies of polyatomic bimolecular reaction dynamics, J. M. Bowman and G. C. Schatz, Annu. Rev. Phys. Chem. **46**, 169-195 (1995).
326. Calculation of the Photodetachment Spectrum of OHCl⁻ Using Complex L^2 Functions, R. C. Mayrhofer and J. M. Bowman, J. Chem. Phys. **102**, 5598-5604 (1995).
327. Reduced dimensionality theory of diatom-diatom reactive scattering, J.M. Bowman and D.-S Wang, in Advances in Molecular

Vibrations and Collision Dynamics, Vol IIB., ed. J. M. Bowman , (JAI, Greenwich, 1994), pp. 187-223.

328. Quantum calculations of unusual mode specificity in $\text{H} + \text{C}_2\text{H}_2 \rightarrow \text{H}_2 + \text{CCH}$, D. Wang and J. M. Bowman, J. Chem. Phys. **101**, 8646-8662 (1994).
329. Collision induced isomerization of a semi-rigid bender hydrogen cyanide, B. L. Lan and J. M. Bowman, J. Chem. Phys. **101**, 8564-8571 (1994).
330. Coupled-channel scattering calculations of $\text{ICN}(\tilde{\text{A}} - \tilde{\text{X}})$ photodissociation using *ab initio* potentials, J. M. Bowman, R. Mayrhofer, Y. Amatatsu J. Chem. Phys., **101**, 9469-9479 (1994).
331. Coupled-channel scattering calculations of rotational resonances of $\text{ArHO}(2\Sigma^+, v=0)$, Baiyu Pan, J. M. Bowman, and Bela Gazdy, Chem. Phys. Lett. **221**, 117-120 (1994).
332. New reduced dimensionality calculations of the $\text{H} + \text{H}_2$ and $\text{D} + \text{H}_2$ reactions, D. Wang and J. M. Bowman, J. Phys. Chem. **98**, 7994-7999 (1994).
333. Test of an adiabatic treatment of rotation for vibration/rotation energies of polyatomic molecules, J. M. Bowman, Chem. Phys. Lett. **217**, 36-40 (1994).
334. Application of complex L^2 functions to the calculation of photodissociation processes , R. Mayrhofer and J.M. Bowman, J. Chem. Phys. **100**, 7229-7238 (1994).
335. L^2 calculations of resonances and final rotational distributions for $\text{HCO}^+\text{H} + \text{CO}$, D. Wang and J.M. Bowman, J. Chem. Phys. **100**, 1021-1027 (1994).
336. Time-dependent quantum study of the HCN^+HNC isomerization, B.L. Lan and J.M. Bowman, J. Phys. Chem. **97**, 12535-12540 (1993).
337. Accurate quartic force fields and vibrational frequencies for HCN and HNC , T.J. Lee, C.E. Dateo, B. Gazdy, and J.M. Bowman, J. Phys. Chem. **97**, 8937-8943 (1993).
338. *Ab initio* calculation of a global potential, vibrational energies, and wave functions for hydrogen cyanide/hydrogen isocyanide, and a simulation of the $\sim\text{A} \sim \text{X}$ emission spectrum., J.M. Bowman, B. Gazdy, J.A. Bentley, T.J. Lee, and C.E. Dateo, J. Chem. Phys. **99**, 308-323 (1993).
339. An adiabatic-bend-Franck-Condon model for rotational distributions in the reaction $\text{H} + \text{H}_2\text{O}$ and $\text{H} + \text{D}_2\text{O}$, D. Wang and J.M. Bowman, Chem. Phys. Lett. **207**, 227-235 (1993).
340. Quantum calculations of mode specificity in reactions of H with HOD and H_2O , D.Wang and J.M. Bowman, J. Chem. Phys. **98**, 6235-6247 (1993).

341. Variational calculations of bound and quasibound states of HCO(J=0 and 1) and comparison with experiment, J.M. Bowman and B. Gazdy, Chem. Phys. Lett. **200**, 311-317 (1992).
342. A global *ab initio* potential for HCN/HNC, exact vibrational energies, and comparison to experiment, J.A. Bentley, J.M. Bowman, B. Gazdy, T.J. Lee, and C.E. Dateo, Chem. Phys. Lett. **198**, 563-569 (1992).
343. Mode selectivity in reactions of H with HOD(100), HOD(001) and HOD(002), J.M. Bowman and D-S. Wang, J. Chem. Phys. **96**, 7852-7854 (1992).
344. Reduced dimensionality quantum calculations of mode specificity in the OH+H₂ $\leftrightarrow$ H₂O reaction, D-S. Wang, and J.M. Bowman, J. Chem. Phys. **96** 8906-8913 (1992).
345. The addition and dissociation reaction H + CO $\leftrightarrow$ HCO. 3. Implementation of isolated resonance RRKM theory with exact quantum studies for J=0, S-W. Cho, A.F. Wagner, B. Gazdy, and J.M. Bowman, J. Phys. Chem. **95**, 9897-9900 (1991).
346. Isolated resonance decomposition of a multichannel S-matrix: A test from the scattering of H + CO=HCO, S-W. Cho, A.F. Wagner, B. Gazdy, and J.M. Bowman, J. Chem. Phys. **96**, 2812-2818 (1992)
347. Theoretical studies of the reactivity and spectroscopy of H + CO $\rightleftharpoons$ HCO. I. Stabilization and scattering studies of resonances for J=0 on the Harding *ab initio* surface, B. Gazdy, J.M. Bowman, S-W. Cho, and A.F. Wagner, J. Chem. Phys. **96**, 2799-2811 (1992)
348. HN₂ and DN₂ resonance spectra: scattering and stabilization calculations, H. Koizumi, G.C. Schatz, and J.M. Bowman, ACS Symp. Series, **502**, 37-47 (1992).
349. Time dependence of OH overtone relaxation in the hydroperoxyl radical, D. Chapman, J.M. Bowman, and B. Gazdy, J. Chem. Phys. **96**, 1919-1930 (1992).
350. Vibrational calculations and potential determination for ArOH*(v=0,1) and ArOD*(v=0,1), U. Schnupf, J.M. Bowman, and M.C. Heaven, Chem. Phys. Lett. **189**, 487-494 (1992) .
351. An adjusted global potential surface for HCN based on rigorous vibrational calculations, J. M. Bowman and B. Gazdy, J. Chem. Phys. **95**, 6309-6316 (1991).
352. Comment on "Effect of Rotational Quantum States (J=0, 1) on the Tunneling Reaction H₂+H $\rightarrow$ H+H₂ in Parahydrogen Solid at 4.2 K", J.M. Bowman, J. Phys. Chem. **95**, 4921-4922 (1991).
353. Vibrational energies and wavefunctions of high energy localized and floppy states of HO₂, J. M. Bowman, Chem. Phys. Lett. **180**, 249-256 (1991).

354. "Feature Article": Reduced dimensionality theory of quantum reactive scattering, J.M. Bowman, J. Phys. Chem. **95**, 4960-4968 (1991).
355. Theoretical stabilization and scattering studies of resonances in the addition reaction $\text{H} + \text{CO} = \text{HCO}$, B. Gazdy, J.M. Bowman, S-W. Cho, and A.F. Wagner, J. Chem. Phys. **94**, 4192-4194 (1991).
356. Model calculations of electronic excitation of Li adsorbed on LiF(001), Y. Shima and J.M. Bowman, J. Chem. Phys. **94**, 801 (1991).
357. Quantized transition-state, J. M. Bowman, Chem. Eng. News **69**, 2-2 (1991).
358. Reaction pathways, a book review of *Intramolecular Motion and Chemical-Reaction*, edited by I. M. Mills, M. S. Child, and R. A. Marcus, J. M. Bowman, Science **252**, 589-589 (1991).
359. A simple method to adjust potential energy surfaces: Application to HCO, J.M. Bowman and B. Gazdy, J. Chem. Phys. **94**, 816-817 (1991).
360. A truncation/recoupling method for eigenvalues and eigenvectors ideal for parallel computation, J. M. Bowman and B. Gazdy, special issue of Theoretica Chimica Acta on Parallel Computing for Chemical Reactivity, **79**, 215-224 (1991).
361. L^2 approach to the calculation of bound states and resonances in HCO: A case study, *Adv. Mol. Vibrations*, Vol IB., eds. J. M. Bowman and M. A. Ratner, (JAI, Greenwich, 1991), pp.105-137
362. A truncation/recoupling method for basis set calculations of eigenvalues and eigenvectors, J. M. Bowman and B. Gazdy, J. Chem. Phys. **94**, 454-460 (1991)
363. Model-calculations of electronic excitation of Li adsorbed on LiF(001), Y. Shima and J. M. Bowman, J. Chem. Phys. **94**, 801-805 (1991).
364. Calculations of highly excited vibrational energies of $\text{HCN}(n_1, 0, n_3)$: a test of a two-mode model, and comparison with experiment, Chem. Phys. Lett. **175**, 434-440 (1990).
365. Experimental and reduced dimensionality quantum rate coefficients for $\text{H}_2(\text{D}_2) + \text{CN} \rightarrow \text{H}(\text{D})\text{CN} + \text{H}(\text{D})$, Q. Sun, D.L. Yang, N.S. Wang, J.M. Bowman, and M.C. Lin, J. Chem. Phys. **93**, 4730-4739 (1990).
366. A movable basis method to calculate vibrational energies of molecules, J.M. Bowman and B. Gazdy, J. Chem. Phys. **93**, 1774-1784 (1990).
367. A potential Surface for $\text{Ar-OH}(^2\Sigma)$ and $\text{Ar-OD}(^2\Sigma)$: Fitting and Assigning Experimental Data with Rigorous Theory, J.M. Bowman, B. Gazdy, P. Schafer, and M.C. Heaven, J. Phys. Chem. **94**, 2226-2229 (1990).

368. A comparison of scattering and L^2 photodetachment Franck-Condon factors for reduced dimensionality $\text{ClHCl}^- \rightarrow \text{Cl} + \text{HCl} + e^-$, Q. Sun, J. M. Bowman, and B. Gazdy, *J. Chem. Soc. Farad. Trans.* **86**, 1737-1740 (1990).
369. A new functional form for global potentials of floppy molecules, Joel M. Bowman and Pamela Schafer, *J. Mol. Struct.*, special Crawford issue, **224**, 133-139 (1990).
370. Theoretical and experimental rate constants for 2 isotopic modifications of the reaction $\text{H} + \text{H}_2$, J.V. Michael, J.R. Fisher, J.M. Bowman, and Q. Sun, *Science*, **249**, 269-271 (1990).
371. Reduced dimensionality quantum reactive scattering: $\text{H}_2 + \text{CN} \rightarrow \text{H} + \text{HCN}$, Q. Sun and J.M. Bowman, *J. Chem. Phys.* **92**, 5201-5210 (1990).
372. Reduced dimensionality diatom-diatom reactive scattering: Application to a model $\text{H}_2 + \text{A}_2 \rightarrow \text{H} + \text{HA}_2$, Q. Sun and J.M. Bowman, *J. Chem. Phys.* **92**, 1021-1029 (1990).
373. Reduced-Dimensionality Quantum Calculations of the Thermal Rate Coefficient for the $\text{Cl} + \text{HCl} \rightarrow \text{ClH} + \text{Cl}$ Reaction: Comparison with Centrifugal-Sudden Distorted-Wave, Coupled Channel Hyperspherical, and Experimental Results, Q. Sun, J.M. Bowman, G.C. Schatz, J.R. Sharp, and J.N.L. Connor, *J. Chem. Phys.* **92**, 1677-1686 (1990).
374. New reduced dimensionality rate constants for $\text{D} + \text{H}_2(v=0,1)$ and $\text{H} + \text{D}_2(v=0,1)$, J. M. Bowman and Q. Sun, *J. Phys. Chem.* **94**, 718-721 (1990).
375. A method to constrain vibrational energy in quasiclassical trajectory calculations, J. M. Bowman, B. Gazdy, and Q. Sun, *J. Chem. Phys.* **91**, 2859-2862 (1989).
376. Diatom-diatom reactive scattering in hypercylindrical coordinates, Q. Sun and J.M. Bowman, *Int. Journ. Quantum Chem.: Quantum Chem Symp.* **23**, 115-126 (1989).
377. A three-dimensional L^2 simulation of the photodetachment spectra of ClHCl^- and IHI^- , B. Gazdy and J. M. Bowman, *J. Chem. Phys.* **91**, 4615-4624 (1989).
378. A reduced dimensionality L^2 simulation of the photodetachment spectra of ClHCl^- and IHI^- , Joel M. Bowman and Bela Gazdy, *J. Phys. Chem.* **93**, 5129-5135 (1989).
379. New numerical approaches to the solution to the N-well Schrödinger equation, Joel M. Bowman and Andrzej Wierzbicki, *Int. J. Quantum Chem.* **35**, 297-303 (1989).
380. Investigations of transformed mass-scaled Jacobi coordinates for vibrations of polyatomic molecules with application to H_2O , Joel M.

- Bowman, Jose Zuñiga, and Andrzej. Wierzbicki, J. Chem. Phys. **90**, 2708-2713 (1989).
381. Exact vibrational energies of non-rotating H₂O and D₂O using an accurate *ab initio* potential, Joel M. Bowman, Andrzej Wierzbicki and Jose Zuñiga, Chem. Phys. Lett. **150**, 269-274 (1988).
382. Rotational rainbows in high energy H+CO scattering, Bela Gazdy, Qiyan Sun, and Joel M. Bowman, Chem. Phys. Lett. **148**, 512-516 (1988).
383. Application of adiabatic switching to vibrational energies of three-dimensional HCO, H₂O, and H₂CO, Qiyan Sun, Joel M. Bowman, and Bela Gazdy, J. Chem. Phys. **89**, 3124-3130 (1988).
384. GVSCF: A general code to perform vibrational self-consistent field calculations, A. Wierzbicki and J.M. Bowman, Comp. Phys. Comm., special issue on molecular vibrations, ed. J.M. Bowman, **51**, 225-232 (1988).
385. Theoretical studies of the energetics and dynamics of chemical reactions, T.H. Dunning, Jr., L.B. Harding, A.F. Wagner, G.C. Schatz, and J.M. Bowman, Science, **240**, 453-459 (1988).
386. *Ab Initio* simulation of the photoelectron spectra of HCO⁻ and DCO⁻, K.M. Christoffel, J.S. Bittman, and J.M. Bowman, Chem. Phys. Lett., **133**, 525-530 (1987).
387. Reduced dimensionality quantum calculations of O(³P) + H₂, J. M. Bowman, Chem. Phys. Lett. **141**, 545-547 (1987).
388. Classical energy transfer in forced oscillator models of inelastic scattering, Bela Gazdy, Qiyan Sun and Joel M. Bowman, J. Chem. Phys. **87**, 6618-6622 (1987).
389. The addition and dissociation reaction H+CO → HCO, I. Theoretical RRKM studies, Albert.F. Wagner and Joel M. Bowman, J. Phys. Chem. **91**, 5314 (1987).
390. Comparison of reduced dimensionality and accurate cumulative reaction probabilities for O(³P)+H₂ (v=0,1), J. M. Bowman, Chem. Phys. Lett. **141**, 545-547 (1987).
391. Vibrational self-consistent field investigation of adsorbate vibrations: Coupling of atomic adsorbate to a rigid corrugated surface, A. Wierzbicki and J.M. Bowman, Surf. Sci. **191**, 518-528 (1987).
392. A new decomposition of the S-matrix for multichannel resonant scattering, Bela Gazdy and Joel M. Bowman, Phys. Rev. A **36** 3083-3090 (1987).
393. Self-consistent field investigation of vibrations of atomic adsorbates, A. Wierzbicki and J.M. Bowman, J. Chem. Phys. **87**, 2363-2369 (1987).

394. A novel decomposition of the multichannel scattering matrix at resonances, B. Gazdy and J.M. Bowman, Phys. Rev. Lett, **59**, 3-5 (1987).
395. Evidence for a rotational rainbow in inelastic hot atom experiments?, J.M. Bowman and B. Gazdy, J. Chem. Phys. **86**, 3046-3046 (1987).
396. Reaction dynamics for $O(^3P) + HD$. VI. Comparison of TST and reduced dimensionality quantum and quasiclassical isotope effects with experiment, A.F. Wagner and J.M. Bowman, J. Chem. Phys. **86**, 1976-1981 (1987).
397. Reaction dynamics for $O(^3P) + HD$. V. Reduced dimensionality quantum and quasiclassical reaction probabilities and rate constants with an adiabatic incorporation of the bending motion, J.M. Bowman and A.F. Wagner, J. Chem. Phys. **86**, 1967-1975 (1987).
398. Rotational distributions from resonant and direct scattering in $H+CO$ and tests of statistical theories, K.-T. Lee and J. M. Bowman, J. Chem. Phys. **86**, 215-225 (1987).
399. The infrared spectrum of the hydrogen bifluoride anion: Unprecedented variation with level of theory, C.L. Janssen, W.D. Allen, H.F. Schaefer III, and J.M. Bowman, Chem. Phys. Lett. **131**, 352-358 (1986).
400. Rotational distributions from resonances in $H+H_2$, J. M. Bowman, Int'l J. Quant. Chem.: Quantum Chem. Symposium 20, p. 681-687 (1986).
401. Rotational distributions and collision lifetimes in $H+CO$ scattering, K.-T. Lee and J. M. Bowman, J. Chem. Phys. **85**, 6225-6226 (1986).
402. *Ab initio* predictions and experimental confirmation of large tunneling contributions to rate constants and kinetic isotope effects ..., B.C. Garrett, D.G. Truhlar, J.M. Bowman, A.F. Wagner, D. Robie, S. Arepalli, N. Presser and R.J. Gordon, J. Am. Chem. Soc. **108**, 3515-3516 (1986).
403. Evaluation of dynamical approximations for calculating the effect of vibrational excitation on reaction rates. $O + H_2 (n=0,1) \rightarrow OH(n=0,1)+H$, B.C. Garrett, D.G. Truhlar, J.M. Bowman and A.F. Wagner, J. Phys. Chem. **90**, 4305-4311 (1986).
404. Collision lifetime approach to recombination and a new derivation of RRKM theory, J.M. Bowman, J. Phys. Chem. **90**, 3492-3495 (1986).
405. *Ab initio* calculations of electronic and vibrational energies of HCO and HOC, J. M. Bowman, J. S. Bittman, L. B. Harding, J. Chem. Phys. **85**, 911-921 (1986).
406. The self-consistent field approach to polyatomic vibrations, J.M. Bowman, Acc. of Chem. Res. **19**, 202-208 (1986)

407. Coupled channel calculations of resonances in H+CO, H. Romanowski, K.-T. Lee, J.M. Bowman, and L.B. Harding, J. Chem. Phys. **84**, 4888-4893 (1986).
408. Reduced dimensionality theories of quantum reactive scattering: Applications to Mu+H₂, H+H₂, O(³P)+H₂, D₂ and HD, J.M. Bowman and A.F. Wagner, NATO ASI Ser., Ser. C, **170**, 47-76 (1986).
409. Reduced dimensionality quantum calculations of resonances in H+H₂, J.M. Bowman, Chem. Phys. Lett. **124**, 260-263 (1986).
410. J. M. Bowman, Nuclear mean-field theory, Phys. Today. **38** (12), 9-9 (1985).
411. Theoretical characterization of chemical reactions of importance in the oxidation of hydrocarbons: reactions of acetylene with hydrogen and oxygen atoms, T.H. Dunning, L.B. Harding, A.F. Wagner, G.C. Schatz and J.M. Bowman, Comp. *Ab initio* Quantum Chem. Exp. Small Mol., Proc. Symp., 67-94 (1985).
412. A semiclassical calculation of the temperature dependence of inelastic phonon transitions in gas-surface scattering: He/Si(100)-(2x1), S.C. Park and J.M. Bowman, Chem. Phys. Lett. **119**, 275-280 (1985).
413. Vibrational energy levels of formaldehyde, H. Romanowski, J.M. Bowman, and L. Harding, J. Chem. Phys. **82**, 4155-4165 (1985).
414. Inclusion and assessment of Renner-Teller coupling in transition state theory for Π states: Application of O(³P)+H₂, A.F. Wagner, J.M. Bowman, and L.B. Harding, J. Chem. Phys. **82**, 1866-1872 (1985).
415. Infrared linewidths and vibrational lifetimes at surfaces: H on Si (100), J.C. Tully, Y.J. Chabal, K. Raghavachari, J.M. Bowman, and R.R. Lucchese, Phys. Rev. B: Condens. Matter, **31**, 1184-1186 (1985).
416. Reduced dimensionality theories of quantum reactive scattering, J.M. Bowman, Adv. Chem. Phys. **61**, 115 (1985).
417. Classical trajectory-quantum forced oscillator study of gas-surface phonon scattering: He/Si(100)-(2x1), J. Chem. Phys. **81**, 6277-6280 (1984).
418. Reaction dynamics for O(³P)+H₂ and D₂. IV. Reduced dimensionality quantum and quasiclassical rate constants with an adiabatic incorporation of the bending motion, J. M. Bowman, A. F. Wagner, S. P. Walch and T. H. Dunning, J. Chem. Phys. **81** (4), 1739-1752 (1984).
419. Another derivation of the cos θ -law for molecules scattered statistically from surfaces, S.C. Park and J.M. Bowman, Chem. Phys. Lett. **110**, 383-384 (1984).

420. A test of the adiabatic approximation for vibrational energies of H_2O , H. Romanowski and J.M. Bowman, Chem. Phys. Lett **110**, 235-239, (1984).
421. Approximate quantum approaches to the calculation of resonances in reactive and non-reactive scattering, J.M. Bowman, K.-T. Lee, H. Romanowski, and L.B. Harding in the ACS Symposium series 263 Resonances in Electron-Molecule Scattering, van der Waals Complexes, and Reactive Chemical Dynamics, D.G. Truhlar, editor, (ACS, Washington, D.C., 1984), Chapter 4, Vol. 263, pp. 43-62.
422. Model studies of atom and molecule diffusion on surfaces, S.C. Park, and J.M. Bowman, J. Chem. Phys. **80**, 2191-2196 (1984).
423. Quasiclassical trajectory studies of rigid rotor-rigid surface scattering. II. Corrugated surface, S.C. Park and J.M. Bowman, J. Chem. Phys. **80**, 2183-2190 (1984).
424. A model study of the laser-induced stabilization of a collision complex, K.F. Milfeld and J.M. Bowman, Chem. Phys. Lett. **100**, 529-534 (1983).
425. Reduced dimensionality quantum rate constants for the $\text{D}+\text{H}_2$ ($v=0$) and $\text{D}+\text{H}_2$ ($v=1$) reactions on the LSTH surface, J.M. Bowman, K.T. Lee and R.B. Walker, J. Chem. Phys. **79**, 3742-3745 (1983).
426. Rotational cooling of rigid rotors desorbed from flat surfaces, J.M. Bowman and J.L. Gossage, Chem. Phys. Lett. **96**, 481-484 (1983).
427. Complex coordinate calculations of Feshbach resonance energies and widths for a collinear triatomic system, K.M. Christoffel and J.M. Bowman, J. Chem. Phys. **78**, Part II, 3952-3958 (1983).
428. Reduced dimensionality quantum calculations of integral cross sections for $\text{H}+\text{H}_2$ ($v=1$) $\rightarrow$ H_2 ($v'=0$), H_2 ($v'=1$)+H, J.M. Bowman and K.T. Lee, Chem. Phys. Lett. **94**, 363-365 (1983).
429. Introduction, J.M. Bowman in Topics in Current Physics, Volume 33: Molecular Collision Dynamics, (J.M. Bowman, ed., Springer, Berlin, 1983) Chapter 1.
430. Rotational Rainbows in Atom-Diatom Scattering, R. Schinke and J.M. Bowman in Topics in Current Physics, Volume 33: Molecular Collision Dynamics, (J.M. Bowman, ed., Springer, Berlin, 1983) Chapter 4.
431. Quasiclassical trajectory studies of rigid rotor-rigid surface scattering. I. Flat surface, J.M. Bowman and S.C. Park, J. Chem. Phys. **77**, 5441-5449 (1982).
432. Incorporation of collinear exact quantum reaction probabilities into three-dimensional transition-state theory, J.M. Bowman, G.-Z. Ju, and K.T. Lee, J. Phys. Chem. **86**, 2232-2239 (1982).

433. *Ab initio* calculation of the transition-state properties and addition rate constants for $\text{H}+\text{C}_2\text{H}_2$ and selected isotopic analogues, L.B. Harding, A.F. Wagner, J.M. Bowman, G.C. Schatz, and K. Christoffel, *J. Phys. Chem.* **86**, 4312-4327 (1982).
434. Approximate quantum differential cross sections for the $\text{F}+\text{HD}\rightarrow\text{HF}+\text{D}$ and $\text{DF}+\text{H}$ reactions, K.T. Lee and J.M. Bowman, *J. Phys. Chem.* **86**, 2289-2291 (1982).
435. Complex coordinate, self-consistent field calculations of vibrational resonance energies, K.M. Christoffel and J.M. Bowman, *J. Chem. Phys.* **76**, 5370-5374 (1982).
436. A comparative study of the reaction dynamics of the $\text{O}(^3\text{P})+\text{H}_2\rightarrow\text{OH}+\text{H}$ reaction on several potential energy surfaces. III. Collinear exact quantum transmission coefficient correction of transition state theory, K.T. Lee, J.M. Bowman, A.F. Wagner, and G.C. Schatz, *J. Chem. Phys.* **76**, 3583-3596 (1982).
437. 47. A comparative study of the reaction dynamics of several potential energy surfaces for $\text{O}(^3\text{P})+\text{H}_2\rightarrow\text{OH}+\text{H}$. II. Collinear exact quantum and quasiclassical reaction probabilities, K.T. Lee, J.M. Bowman, A.F. Wagner, and G.C. Schatz, *J. Chem. Phys.* **76**, 3563-3582 (1982).
438. Approximate quantum differential cross sections for the $\text{F}+\text{H}_2$ reaction, J.M. Bowman, K.-T. Lee, and G.-Z. Ju, *Chem. Phys. Lett.* **86**, 384-388 (1982).
439. Quasitrapping and rainbow mechanisms in model rigid-rotor-rigid-surface scattering, J.M. Bowman and S. Park, *J. Chem. Phys.* **76**, 1168-1170 (1982).
440. Investigations of self-consistent field, SCF CI and virtual state configuration interaction vibrational energies for a model three-mode system, K.M. Christoffel and J.M. Bowman, *Chem. Phys. Lett.* **85**, 220-224 (1982).
441. New approximate quantum cross sections for the $\text{H}+\text{H}_2$ reaction, J.M. Bowman, G.-Z. Ju, and K.T. Lee, *J. Chem. Phys.* **75**, 5199-5201 (1981).
442. Tests of collinear quasiclassical trajectory transmission coefficient correction to transition state theory, J.M. Bowman, G.-Z. Ju, K.T. Lee, A.F. Wagner, and G.C. Schatz, *J. Chem. Phys.* **75**, 141-147 (1981).
443. Classical trajectory studies of multiphoton and overtone absorption of HF, K.M. Christoffel and J.M. Bowman, *J. Phys. Chem.* **85**, 2159-2163 (1981).
444. Quantum and classical dynamics of a coupled double well oscillator, K.M. Christoffel and J.M. Bowman, *J. Chem. Phys.* **74**, 5057-5075 (1981).

445. A comparative study of the reaction dynamics of several potential energy surfaces of $O(^3P)+H_2 \rightarrow OH+H$. I. G.C. Schatz, A.F. Wagner, S.P. Walch, and J.M. Bowman, J. Chem. Phys. **74**, 4984-4996 (1981).
446. The evaluation of fitting functions for the representation of an $O(^3P)+H_2$ potential energy surface. I A.F. Wagner, G.C. Schatz, and J.M. Bowman, J. Chem. Phys. **74**, 4960-4983 (1981).
447. Reply to comment by Thomas on "-2665 in inelastic molecular collisions," J.M. Bowman and K.T. Lee, J. Chem. Phys. **74**, 2664 (1981).
448. Exact quantum reaction probabilities for $O(^3P)+H_2$ reaction on an *ab initio* and diatomics-in-molecules potential energy surface, J.M. Bowman and K.T. Lee in Potential Energy Surfaces and Dynamic Calculations, D.G. Truhlar, Ed., (Plenum, New York, 1981), pp. 359-373.
449. Wave vector modification of the infinite order sudden approximation, J.G. Sachs and J.M. Bowman, J. Chem. Phys. **73**, 3699-3708 (1980).
450. Testing and correcting the sudden approximation: Application to rotationally inelastic scattering, J.M. Bowman, K.T. Lee and J.G. Sachs, Chem. Phys. Lett. **74**, 90-94 (1980).
451. Sudden rotation reactive scattering: Theory and application to 3-D $H+H_2$, J.M. Bowman and K.T. Lee, J. Chem. Phys. **72**, 5071-5088 (1980).
452. An SCF-State interaction method for coupled oscillator systems, F. Tobin and J.M. Bowman, Chem. Phys. **47**, 151-159 (1980).
453. Sudden approximation theory of vibrational excitation, J.M. Bowman, Int. J. Quantum Chem.: Quantum Chem. Symposium, **13**, 487-500 (1979).
454. A test of the quantum mechanical sudden vibrational approximation for collinear inelastic collisions, J.M. Bowman, G. Drolshagen, and J.P. Toennies, J. Chem. Phys. **71**, 2270-2274 (1979).
455. Sudden rotation calculations of the $H+H_2(v=1, j=0)$ reaction, J.M. Bowman and K.T. Lee, Chem. Phys. Lett. **64**, 291-294 (1979).
456. Application of SCF-SI theory to vibrational motion in polyatomic molecules, J.M. Bowman, K. Christoffel, and F. Tobin, J. Phys. Chem. **83**, 905-912 (1979).
457. Rotational rainbows in inelastic atom-molecule differential cross sections, J.M. Bowman, Chem. Phys. Lett. **62**, 309-311 (1979).
458. Tests of semiclassical theory for rotationally inelastic scattering, J.M. Bowman and K.-T. Lee, Chem. Phys. Lett. **60**, 212-215 (1979).

459. Sudden approximation calculations of reactive scattering: The H+H₂ reaction, J.M. Bowman and K.T. Lee, J. Chem. Phys. **68**, 3940-3941, (1978).
460. Deactivation pathways in collisions of Kr with CO₂(001), J.M. Bowman and S. Leasure, Chem. Phys. Lett. **56**, 183-185, (1978).
461. Laplace transformation of the Schrödinger equation: Application to scattering, S. Leasure and J.M. Bowman, J. Chem. Phys. **68**, 2825-2830, (1978).
462. Self-consistent field energies and wavefunctions for coupled oscillators, J.M. Bowman, J. Chem. Phys. **68**, 608-610, (1978).
463. Fully converged sudden rotation total integral cross sections for ⁴He + H₂ (v=0, j=0)→⁴He + H₂ (v'=1, j'), S.C. Leasure and J.M. Bowman, Chem. Phys. Lett. **48**, 179-183, (1977).
464. An improved quasiclassical histogram method, J.M. Bowman and S.C. Leasure, J. Chem. Phys. **66**, 1756-1757, (1977).
465. Quasiclassical studies of rigid rotor-solid surface diffraction scattering, C.J. Ray and J.M. Bowman, J. Chem. Phys. **66**, 1122-1126, (1977).
466. Sudden rotation total rotational inelastic cross sections for ⁴He + I₂^{*}, J.M. Bowman, J. Chem. Phys. **66**, 296-297, (1977).
467. Sudden rotation calculations of atom-molecule scattering, J.M. Bowman and S.C. Leasure, J. Chem. Phys. **66**, 288-295, (1977).
468. Large quantum effects in a model electronically nonadiabatic reaction: Ba + N₂O→BaO^{*} + N₂, J.M. Bowman, S.C. Leasure and A. Kuppermann, Chem. Phys. Lett. **43**, 374-376, (1976).
469. Static rotation and quasiclassical total cross sections for atom-rigid rotor scattering: ⁴He + I₂ (j=12)→⁴He + I₂ (j') J.M. Bowman and J. Arruda, Chem. Phys. Lett. **41**, 43-45, (1976).
470. On the use of an adiabaticity criterion to reduce computation time in quasiclassical trajectory calculations, J. Chem. Phys. **64**, 4229-4230, (1976).
471. A dynamic threshold in the F + H₂ → HF + H reaction as determined from three-dimensional quasi-classical-reverse trajectory calculations, S.C. Leasure and J.M. Bowman, Chem. Phys. Lett. **39**, 462-467, (1976).
472. Quasiclassical trajectory calculations of He-LiF (001) diffraction scattering, C.J. Ray and J.M. Bowman, J. Chem. Phys. **63**, 5231, (1975).
473. A semi-numerical approach to the construction and fitting of triatomic potential energy surfaces, J.M. Bowman and A. Kuppermann, Chem. Phys. Lett. **34**, 523-527, (1975).

474. Exact quantum, quasiclassical, and semiclassical reaction probabilities for the collinear $F+D_2 \rightarrow FD+D$ reaction, G.C. Schatz, J.M. Bowman and A. Kuppermann, J. Chem. Phys. **63**, 685-696, (1975).
475. Exact quantum, quasiclassical, and semiclassical reaction probabilities for the collinear $F+H_2 \rightarrow FH+H$ reaction, G.C. Schatz, J.M. Bowman and A. Kuppermann, J. Chem. Phys. **63**, 674-684, (1975).
476. Violation of microscopic reversibility and the use of reverse quasi-classical trajectories for calculating reaction cross sections, J.M. Bowman, G.C. Schatz and A. Kuppermann, Chem. Phys. Lett. **24**, 378-380, (1974).
477. Comparison of semiclassical, quasiclassical, and exact quantum transition probabilities for the collinear $H+H_2$ exchange reaction, J.M. Bowman and A. Kuppermann, J. Chem. Phys. **59**, 6524-6534, (1973).
478. Semi-classical S matrix theory of reactive and non-reactive atom-molecule collisions, J.M. Bowman and A. Kuppermann, Chem. Phys. **2**, 158-170, (1973).
479. A direct test of the vibrationally adiabatic theory of chemical reactions, J.M. Bowman, A. Kuppermann, J.T. Adams and D.G. Truhlar, Chem. Phys. Lett. **20**, 229-232, (1973).
480. Large quantum effects in the collinear $F+H_2 \rightarrow FH+H$ reaction, G.C. Schatz, J.M. Bowman and A. Kuppermann, J. Chem. Phys. **58**, 4023-4025, (1973).
481. Comparison of semi-classical, exact quantum, and quasi-classical reactive transition probabilities for the collinear $H+H_2$ reaction, J.M. Bowman and A. Kuppermann, Chem. Phys. Lett. **19**, 166-170, (1973).
482. Quantum initial conditions in quasi-classical trajectory calculations, J.M. Bowman, A. Kuppermann and G.C. Schatz, Chem. Phys. Lett. **19**, 21-25, (1973).
483. Classical and quantum reaction probabilities and thermal rate constants for the collinear $H+H_2$ exchange reaction with vibrational excitation, J.M. Bowman and A. Kuppermann, Chem. Phys. Lett. **12**, 1-4, (1971).