Comparisons of sets of electron-neutral scattering cross sections and calculated swarm parameters in Kr and Xe

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Introduction

Xenon is used in a number of application areas ranging from light sources to x-ray detectors for imaging in medicine, border security and high-energy particle physics. There is a correspondingly large body of data available for electron scattering cross sections and swarm parameters in Xe, whereas data for Kr are more limited. In this communication we show intercomparisons of the cross section sets in Xe and Kr presently available on the LXCat site. **Swarm parameters** calculated using these cross sections sets are compared with experimental data, also available on the LXCat site. As was found for Ar, diffusion coefficients calculated using these cross section data in a 2-term Boltzmann solver are higher than Monte Carlo results by about 30{\%} over a range of E/N from 1 to 100 Td. We find otherwise good agreement in Xe between **2-term** and **Monte Carlo** results and between measured and calculated values of electron mobility, ionization rates and light emission (dimer) at atmospheric pressure. The available cross section data in Kr yield swarm parameters in agreement with the limited experimental data. The cross section compilations and measured swarm parameters used in this work are available on-line at www.lxcat.laplace.univ-tlse.fr.

"Complete" sets of cross sections available on LXCat for electron scattering from Krypton and Xenon

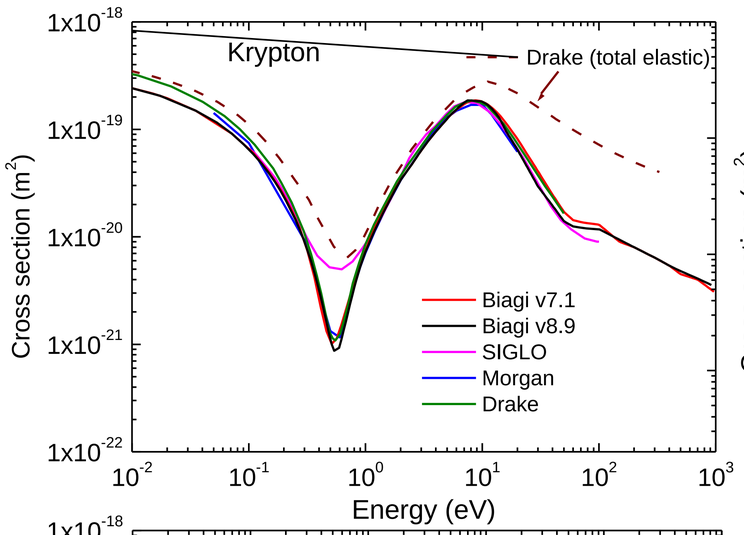
Kr

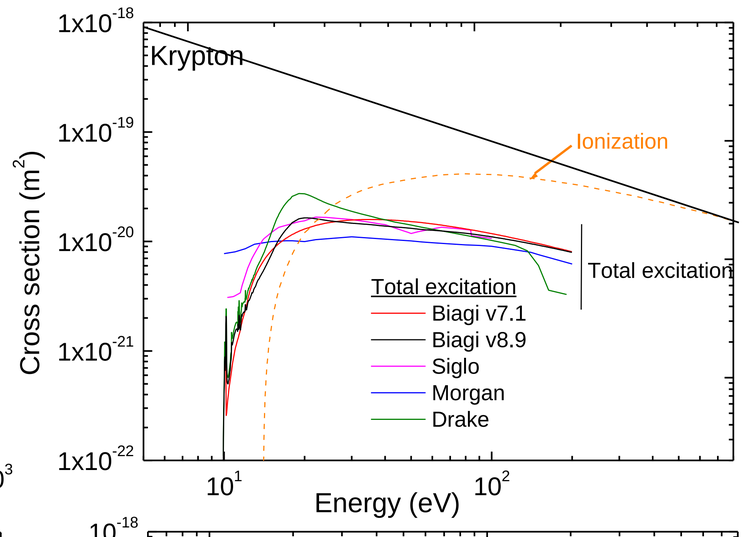
Database	Level of detail for excitation	Comments
SIGLO	**5 levels**	For use in a 2-term Boltzmann solver. From Date et al., J. Phys. D 22, 1478 (1989)
Morgan	**2 levels**	For use in a 2-term Boltzmann solver.
Biagi -v7.1	**3 excitation levels (S,P & D+P)**	For use with Monte Carlo or multi-term Boltzmann solvers
Biagi -v8.97	**51 levels**	For use with Monte Carlo or multi-term Boltzmann solver. Based in part on quantum calculations of Zatsarinny and Bartschat
Drake (O Zatsarinny and K Bartschat)	**68 levels**	Results of quantum calculations. From Allan et al. , J. Phys. B 44, 065201 (2011) Cross section for ionization is not included.

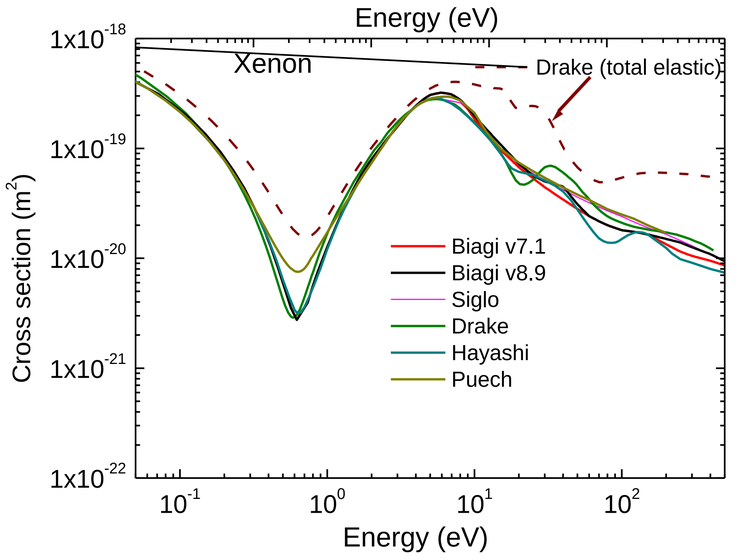
Xe

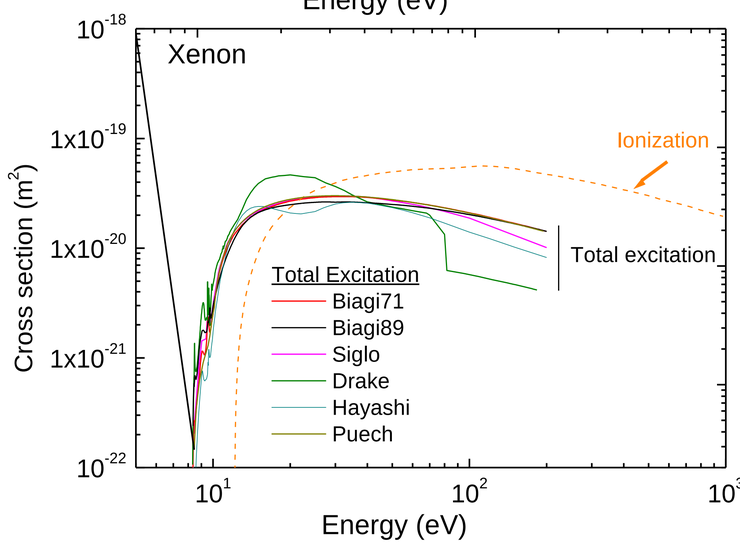
Database	Level of detail for excitation	Comments
SIGLO	**6 levels;**	For use with a multiterm Boltzmann solver. From Meunier et al. J. Appl. Phys. 78, 731 (1995)
Morgan	**2 levels (metastable + resonance)**	For use in a 2-term Boltzmann solver. Note : the limited energy range for the elastic momentum transfer cross section precludes using these cross sections for calculations in pure xenon.
Biagi v7.1	**4 levels**	For use with Monte Carlo or multi-term Boltzmann solver.
Biagi v8.97	**50 levels**	For use with Monte Carlo or multi-term Boltzmann solver.
Puech	**13 levels**	For use with a 2-term boltzmann solver. Puech and Mizzi, J. Phys. D 24, 1974 (1991)
Hayashi	**14 levels**	For use with Monte Carlo of multi-term Boltzmann solvers. See report NIFS-DATA-79 (2003).
Drake (O Zatsarinny and K Bartschat)	**74 levels**	Results of quantum calculations. From Allan et al. , J. Phys. B 43, 074031 (2010) Cross section for ionization is not included.

Databases containing cross sections





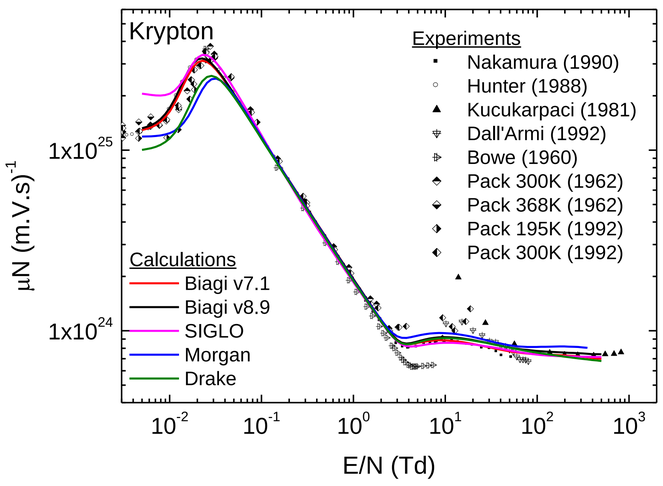


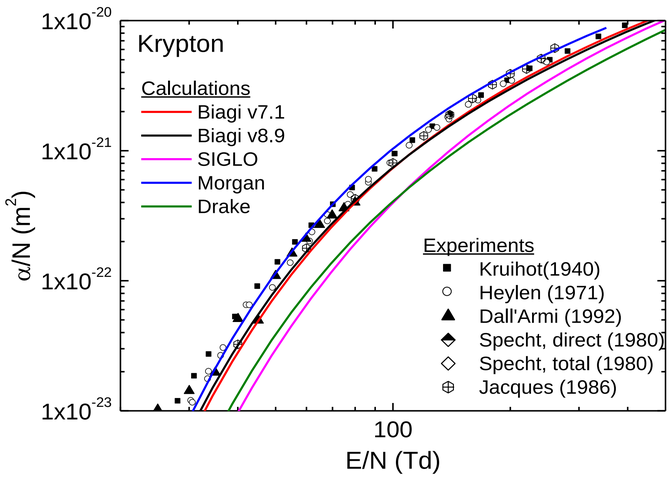


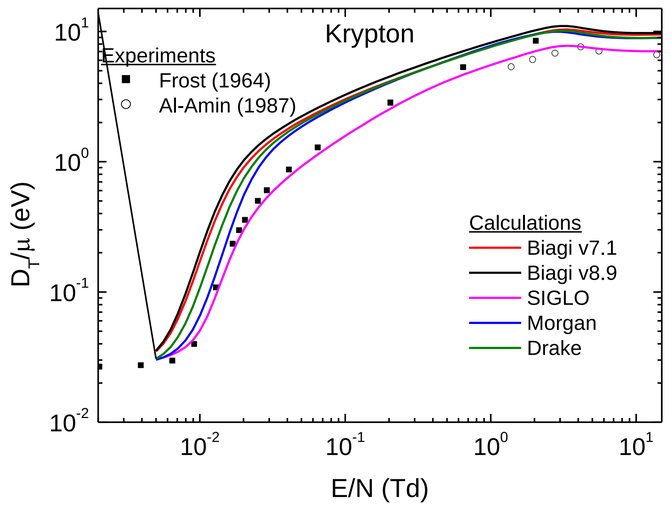
Transport and rate coefficients calculated using LXCat input data and comparisons with experiment

These calculations were performed using BOLSIG+, a 2-term Boltzmann solver, with a spatial growth model (SST)

Kr







Characteristic energy, **D_T/μ, vs E/N**

Xe

Mobility x neutral gas density, **μN vs. E/N**
For full range of experimental data, see **LXCat**.

Ionization rate, **α/N vs. E/N**

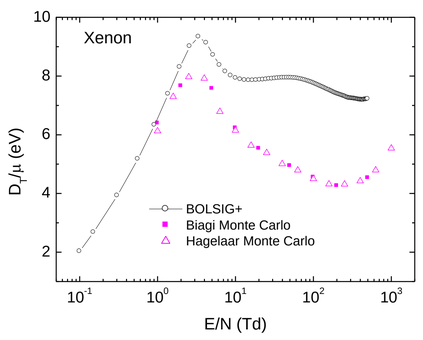
Conclusions

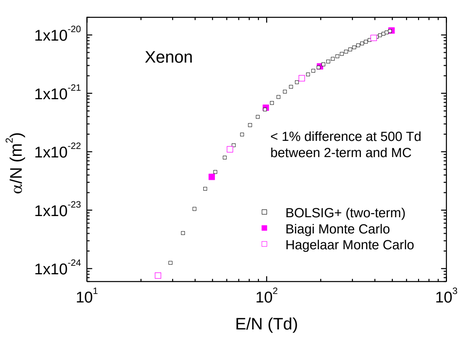
• Precision data are lacking for the mobility (drift velocity) above about 50 Td in Xe and Kr. The drift velocity in this region is sensitive to the peak of the elastic momentum transfer cross section. More guidance from experiment is needed here.

• Penning effects influence the ionization coefficient in the low E/N range and more experiments are needed here, too.

• For high precision calculations, should be taken to use the cross section sets in either two-term Boltzmann or in Monte Carlo simulations or multi-term Boltzmann solvers.

Intercomparison of Boltzmann and Monte Carlo codes





The two-term approximation yields accurate values for mobility and ionization rates in Kr and Xe, but the uncertainty in the predicted characteristic energy , D_T/μ is large as shown above. Similar behavior is found in the other rare gases with Ramsauer minima, with the largest uncertainty being in Xenon.

References for codes :

- 2-term Boltzmann : Hagelaar, BOLSIG+ (full version downloadable from LXCat site)
- Biagi Monte Carlo : Magboltz (available from the CERN website)