

# **ADAS8#3 for Automated $R$ -matrix calculations**

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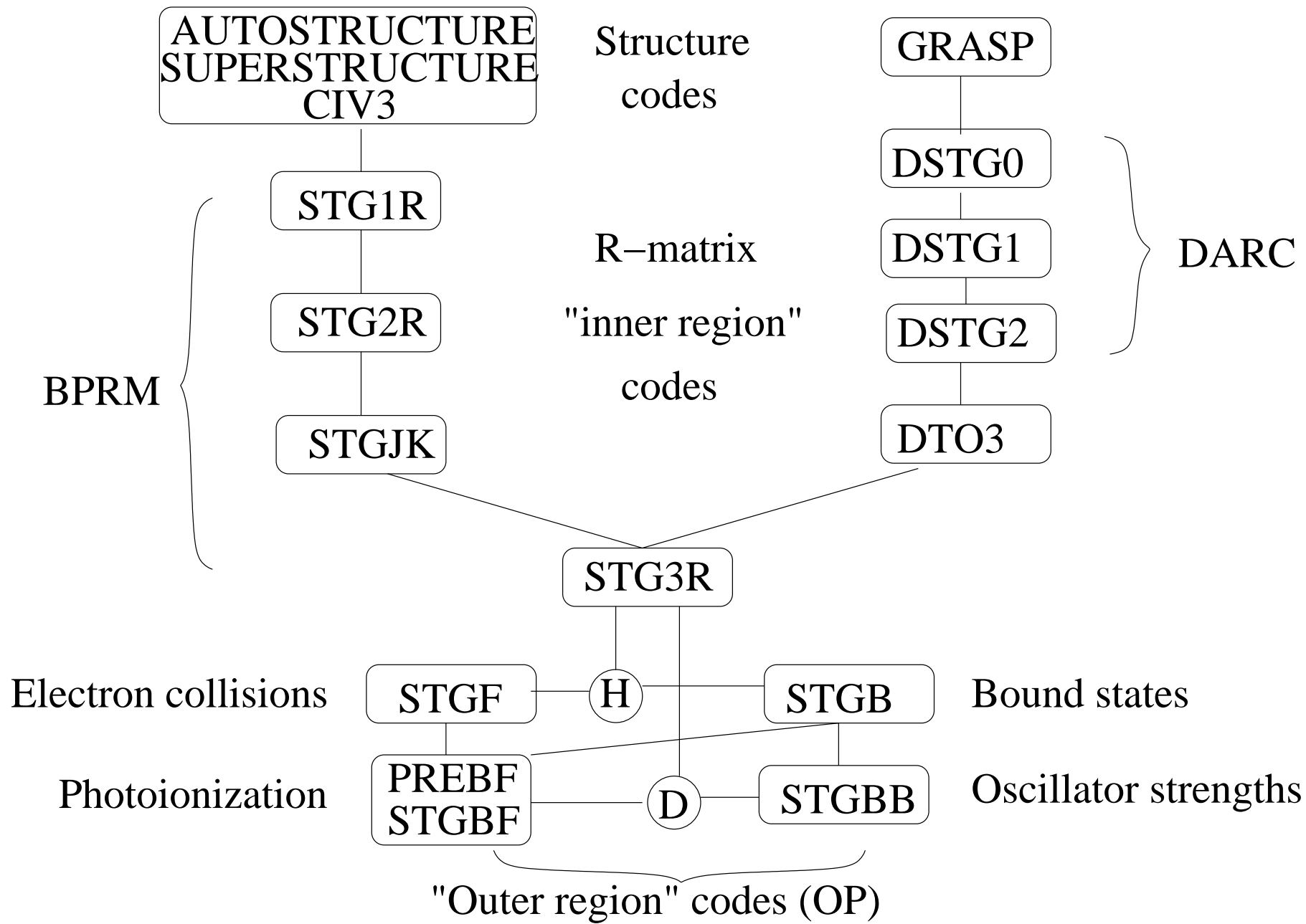
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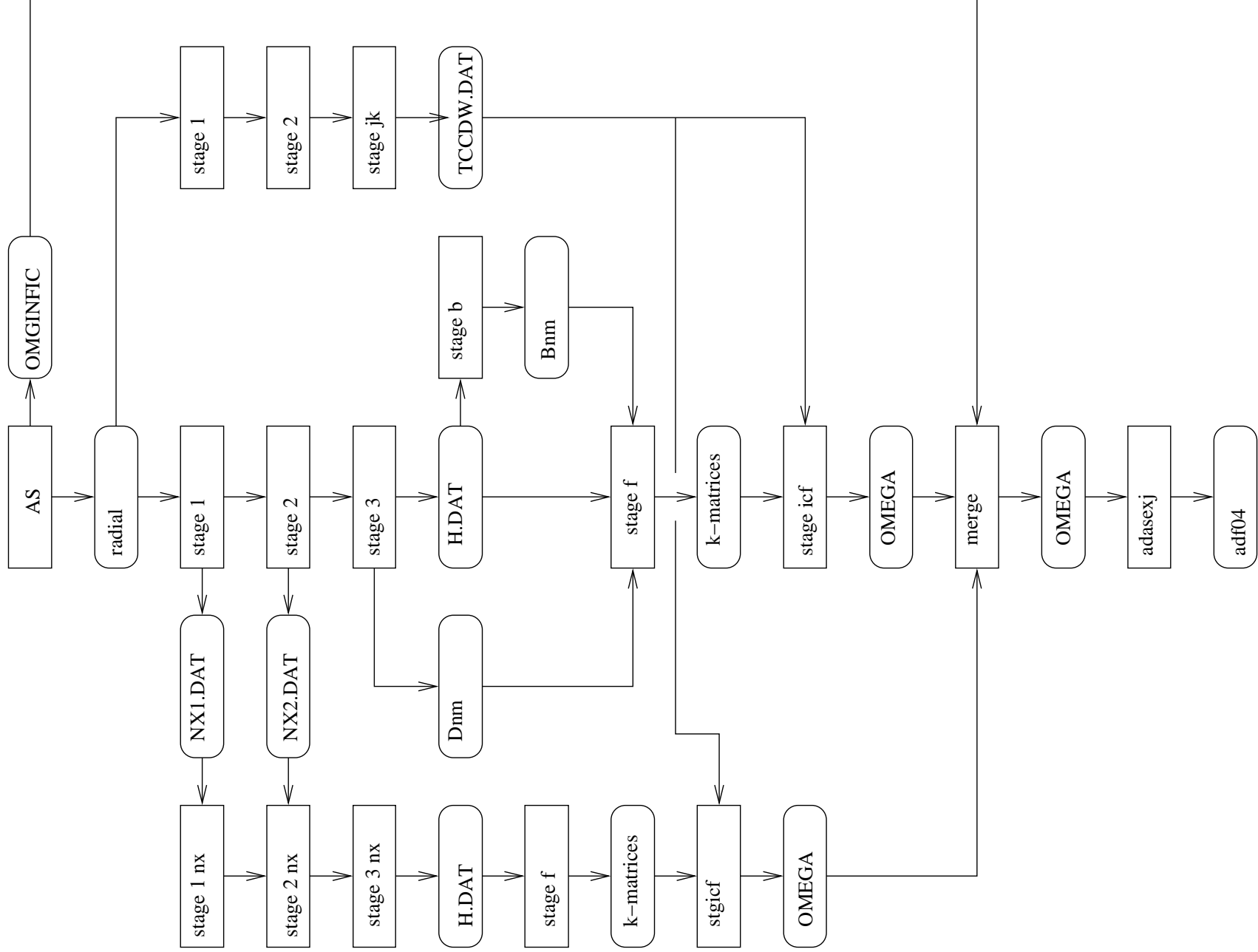
# Contents

Very brief talk — almost an announcement.

- How  $R$ -matrix calculations by non-experts usually go.
- ADAS8#3.
- Example input.
- Current and future work.

**How  $R$ -matrix calculations  
usually go...**





S.S.

&STG2A RELOP='MVD' ISORT=1 &END

&STG2B MAXORB=6 NELC=7 NAST=120 INAST=0 MINLT=0 MAXLT=13 MINST=1 MAXST=7 &END

1 0 2 0 2 1 3 0 3 1 3 2

12

2 0 2 0 0 0

2 2 5 1 1 1

2 2 3 0 0 0 0

2 1 4 0 0 0 0

2 0 5 0 0 0 0

2 2 2 1 0 0 0

2 2 2 0 1 0 0

2 2 2 0 0 1 0

2 1 3 1 0 0 0

2 1 3 0 1 0 0

2 1 3 0 0 1 0

2 0 4 1 0 0 0

2 0 4 0 1 0 0

2 0 4 0 0 1 0

4 0 1

2 2 1

2 1 1

4 1 0 &STGF IMESH=1 IQDT=2 PERT='YES' IPRINT=-2

2 2 0 IPRKM=4 IRDO=101 NOMWRT=-50 &END

2 0 0 &MESH1 MXE=1000 E0=0.3215141 EINCR=5e-05 &END

2 1 0

2 1 1 C

4 1 0 &STGIC ITCC=1 IMODE=0 INOEXCH=0 NOMWRT=-9999999 IRDO=50 PRINT='UNFORM' &END

2 1 0 &MESH1 MXE=1000 E0=0.3215141 EINCR=5e-05 &END

2 2 0

...

A.S.

&SALGEB RAD='ALL' CUP='ICM' MXVORB=5 MXCONF=12 KUTSO=0

BORN='INF' KORB1=1 KORB2=1 &END

2 0 2 1 3 0 3 1 3 2

2 3 0 0 0

1 4 0 0 0

0 5 0 0 0

2 2 1 0 0

2 2 0 1 0

2 2 0 0 1

1 3 1 0 0

1 3 0 1 0

1 3 0 0 1

0 4 1 0 0

0 4 0 1 0

0 4 0 0 1

&SMINIM NZION=12 INCLUD=0 NLAM=6 PRINT='FORM' RADOUT='YES' &END

S.S.

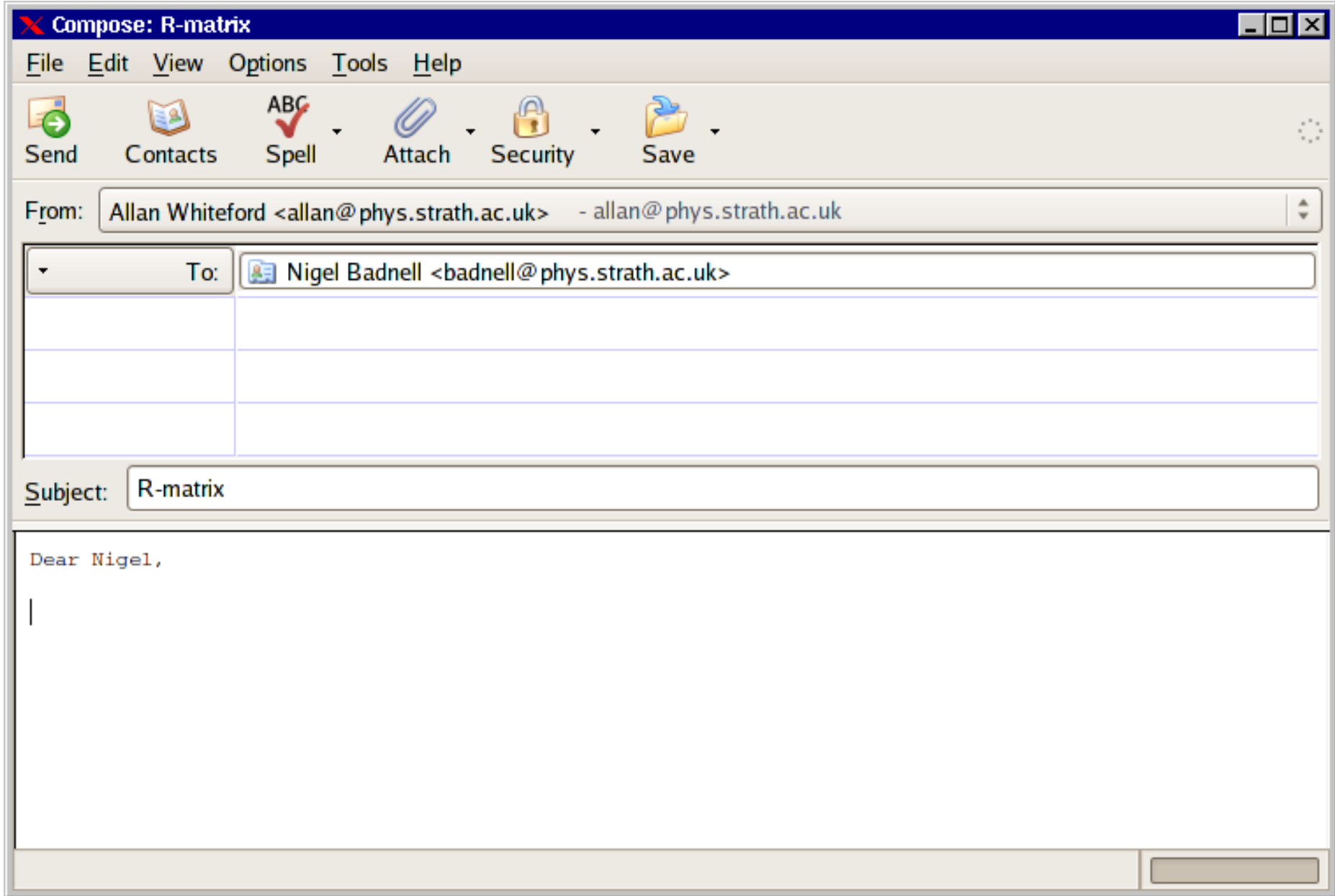
&STG1A RELOP='MVD' &END

&STG1B MAXLA=4 MAXLT=13 MAXC=20 MAXE=44 &END

S.S.

&STG3A &END

&STG3B INAST=0 NAST=0 &END



## ADAS8#3

- Designed to automatically generate input files and run codes.
- Produces fully **documented** adf04 file with *R*-matrix collision strengths and AUTOSTRUCTURE *A*-values.
- Makes 'easy' (e.g. He-like systems) calculations straightforward.
- Speeds up handle-turning.
- Doesn't remove need for expert in advanced calculations.
- Currently limited to ICFT based calculations.
- Part of offline-ADAS suite of codes.



## Example input

### CONFIGURATION LIST

1s2 2s2 2p3

1s2 2s1 2p4

1s2 2p5

1s2 2s2 2p2 3s1

1s2 2s2 2p2 3p1

1s2 2s2 2p2 3d1

1s2 2s1 2p3 3s1

1s2 2s1 2p3 3p1

1s2 2s1 2p3 3d1

1s2 2p4 3s1

1s2 2p4 3p1

1s2 2p4 3d1

## Usage so far and further work

- So far:
  - Full F-like iso-electronic sequence\*,
  - Full He-like iso-electronic sequence,
  - Works at Strathclyde on three computer systems,
  - Some work at Catania,
  - Will run on a laptop!
- Further work:
  - Full Li-like iso-electronic sequence,
  - Full H-like iso-electronic sequence,
  - DARC and full BP code integration,
  - Hopefully everything up to Mg-like in the next 3–5 years.

\* M C Witthoef, A D Whiteford and N R Badnell *J. Phys. B.* **40** 2969