

ADAS Subroutine gext

```
FUNCTION GEXT(X,N,L)
  IMPLICIT REAL*8 (A-H,O-Z)
```

C

```
C PURPOSE: PRODUCES ONE ELECTRON ORBITALS FROM SPECIFIED
C           FUNCTIONAL FORMS
```

C

```
C FOR USE IN DWBES, RDWBES,DWDIP WITH EXTERNAL OPTION IEXT=1
```

C

```
C HIBBERT (CIV3 PROGRAM) ORBITALS FOR OII 24/4/85
```

C

```
C INDEXING OF WAVE FUNCTIONS BY I=(N*(N-1))/2+L+1
```

```
C UNIX-IDL PORT:
```

C

```
C-----
```

```
C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
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```
C DATE: 4TH JULY 1996
```

C

```
C VERSION: 1.1 DATE: 04-07-96
```

```
C MODIFIED: WILLIAM OSBORN
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```
C           - FIRST VERSION.
```

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```
C VERSION: 1.2 DATE: 20-07-07
```

```
C MODIFIED: Allan Whiteford
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C           - Small modification to comments to allow for
C           automatic documentation preparation.
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C

```
      I=(N*(N-1))/2+L+1
```

```
      GO TO (1,2,3,4,5,6),I
```

```
1  GEXT=X*(38.1978304D0*DEXP(-7.4780300*X)+4.9817906D0*DEXP(-12.6307
&000D0*X))+X*X*(0.0928714D0*DEXP(-3.1009000D0*X)+2.1368144D0*DEXP(-
&6.3727700D0*X)-0.0087901D0*DEXP(-2.0732300D0*X))
```

```
      RETURN
```

```
2  GEXT=X*(-9.6934267D0*DEXP(-7.4780300D0*X)-0.5036558D0*DEXP(-12.63
&07000D0*X))+X*X*(9.2494101D0*DEXP(-3.1009000D0*X)-11.2771775D0*DEX
&P(-6.3727700D0*X)+4.5358980D0*DEXP(-2.0732300D0*X))
```

```
      RETURN
```

```
3  GEXT=X*X*(4.5603425D0*DEXP(-2.2378000D0*X)+7.9197229D0*DEXP(-3.82
&44700D0*X))+1.1697093D0*DEXP(-1.6770200D0*X)+2.6575680D0*DEXP(-8.58
&10500D0*X))
```

```
      RETURN
```

```
4  GEXT=X*(3.7467103D0*DEXP(-6.4449722D0*X))+X*X*(-5.0254465D0*DEXP(
&-2.4960885D0*X))+X*X*X*(0.5162317D0*DEXP(-1.0396983D0*X))
```

```
      RETURN
```

```
5  GEXT=X*X*(4.0687494D0*DEXP(-2.6750348D0*X))+X*X*X*(-0.2285374D0*D
&EXP(-0.8361112D0*X))
```

```
      RETURN
```

```
6  GEXT=X*X*X*(0.1289291D0*DEXP(-0.7128119D0*X))
```

```
      RETURN
```

```
END
```

```
INTEGER
```

```
L,
```

```
N
```

REAL*8

X