Example 3.5.3.2. *Multipole expansion for an atom in the proton sponge complex of Example 3.5.3.1.*

```
loop_
_atom_rho_multipole_atom_label
_atom_rho_multipole_coeff_Pv
_atom_rho_multipole_coeff_P00
_atom_rho_multipole_coeff_P11
_atom_rho_multipole_coeff_P1-1
_atom_rho_multipole_coeff_P10
_atom_rho_multipole_coeff_P20
_atom_rho_multipole_coeff_P21
_atom_rho_multipole_coeff_P2-1
_atom_rho_multipole_coeff_P22
_atom_rho_multipole_coeff_P2-2
_atom_rho_multipole_coeff_P30
_atom_rho_multipole_coeff_P31
_atom_rho_multipole_coeff_P3-1
_atom_rho_multipole_coeff_P32
_atom_rho_multipole_coeff_P3-2
_atom_rho_multipole_coeff_P33
_atom_rho_multipole_coeff_P3-3
_atom_rho_multipole_coeff_P40
_atom_rho_multipole_coeff_P41
_atom_rho_multipole_coeff_P4-1
_atom_rho_multipole_coeff_P42
_atom_rho_multipole_coeff_P4-2
_atom_rho_multipole_coeff_P43
_atom_rho_multipole_coeff_P4-3
_atom_rho_multipole_coeff_P44
_atom_rho_multipole_coeff_P4-4
_atom_rho_multipole_kappa
_atom_rho_multipole_kappa_prime0
_atom_rho_multipole_kappa_prime1
_atom_rho_multipole_kappa_prime2
_atom_rho_multipole_kappa_prime3
_atom_rho_multipole_kappa_prime4
_atom_rho_multipole_configuration
_atom_rho_multipole_radial_slater_n0
_atom_rho_multipole_radial_slater_zeta0
_atom_rho_multipole_radial_slater_n1
_atom_rho_multipole_radial_slater_zeta1
_atom_rho_multipole_radial_slater_n2
_atom_rho_multipole_radial_slater_zeta2
_atom_rho_multipole_radial_slater_n3
_atom_rho_multipole_radial_slater_zeta3
_atom_rho_multipole_radial_slater_n4
_atom_rho_multipole_radial_slater_zeta4
_atom_rho_multipole_core_source
_atom_rho_multipole_valence_source
N(1)    2.63(5)
  0.00       -0.037(17)   0.062(14)   0.00     -0.084(18)
  0.00        0.00       -0.027(15)  -0.048(13)   0.00
 -0.098(16)  -0.063(14)   0.00         0.00       0.082(14)
 -0.037(14)   0.00        0.00         0.00       0.00
  0.00        0.00        0.00         0.00       0.00
0.992(8)      0.80(4)      0.80     0.80     0.80    0.80
;
1S 2S 3S 4S 2P 3P 4P 3D 4D 4F 5S 5P 6S 6P 5D 7S 6D 5F
 2 -2  0  0 -3  0  0  0  0  0  0  0  0  0  0  0  0  0
;
   2   7.2553  2   7.2553  2   7.2553  3   7.2553
   4   7.2553
'Clementi & Roetti, 1974'
'Clementi & Roetti, 1974'

# Data for other atoms have been omitted for brevity
```

a neutral atom. κ is the valence electron expansion factor (`_atom_rho_multipole_kappa`), $R(\kappa'(l), l, \mathbf{r})$ is the radial function (Slater or equivalent) (`_atom_rho_multipole_radial_*`), $\kappa'(l)$ is the multipole function expansion factor (`_atom_rho_multipole_kappa_prime[l]`), $P(l,m)$ are the spherical harmonic coefficients (`_atom_rho_multiple_coeff_P[lm]`) and $d(l,m,\theta,\varphi)$ is the spherical harmonic of order l,m at the angle (θ,φ). The summations are performed over the index ranges $0 \leq l \leq l_{\max}$, $-l \leq m \leq l$, where $l_{\max}$ is the highest order of multipole applied.

Example 3.5.3.2 demonstrates how the category is used in the proton sponge complex of Example 3.5.3.1. Only the first atom is shown in the example.

3.5.4. Development of the dictionary and supporting software

The first implementation of the dictionary appeared in a version of the *XD* program package (Koritsanszky *et al.*, 2003). Thus *XD* can read and write CIFs which include data items in the two categories described above (as well as, of course, items in the core CIF dictionary). It is envisaged that future developments to the rhoCIF dictionary will add features that are relevant to other widely used program packages. In the *XD* implementation, use was made of the *CIFtbx* library of Fortran functions for programming CIF applications (Hall & Bernstein, 1996).

We thank the users of the program package *XD* (Koritsanszky *et al.*, 2003) who provided feedback during the development of the rhoCIF dictionary and Brian McMahon for helpful comments on its presentation.

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