

Generally, all generated descriptors might be spited in two groups:

First category includes attributes such as the maximum row on periodic table, average atomic number and the range of atomic radii between all elements present in the material.

Full list of first type features:

1. *AtomicWeight*
2. *Number*
3. *Column*
4. *Row*
5. *CovalentRadius*
6. *Electronegativity*
7. *GSbandgap*
8. *GSmagmom*
9. *MeltingT*
10. *MendeleevNumber*
11. *SpaceGroupNumber*
12. *GSvolume_pa*

Second category includes electronic structure attributes, which are the average fraction of electrons from the *s, p, d* and *f* (*Ns, Np, Nd* and *Nf* indexes respectively) valence shells between all present elements .

Full list of second type features:

1. *NUnfilled*
2. *NValence*
3. *NdUnfilled*
4. *NdValence*
5. *NfUnfilled*
6. *NfValence*
7. *NpUnfilled*
8. *NpValence*
9. *NsUnfilled*
10. *NsValence*

For all descriptors listed above (first and second category) generated property statistics, which are defined by the following parameters:

1. *minimum*
2. *maximum*
3. *range*
4. *mode*
5. *mean*
6. *mean absolute deviation*

For instance, property *AtomicWeight* has features:

minimum_AtomicWeight, maximum_AtomicWeight, range_AtomicWeight, mode_AtomicWeight, mean_AtomicWeight, avg_dev_AtomicWeight)

Therefore, total number of features is $12 \times 6 = 72$ and $10 \times 6 = 60$ for the first and second category respectively.