|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | n | normalization | exp | l | b | r | m | norm\_adj | Theta | Phi |
| 1s | 1 | 1/sqrt(pi) | -br | 0 | 3/2 | 1 | 0 | 1 | 1 | 1 |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | n | normalization | exp | l | b | r | m | norm\_adj | Theta | Phi |
| 2s | 2 | 1/sqrt(32pi) | -br/2 | 0 | 3/2 | 2-br | 0 | 1 | 1 | 1 |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | n | normalization | exp | l | b | r | m | norm\_adj | Theta | Phi |
| 2py |  |  |  | 1 | 5/2 | r | -1 | 1 | Sin | Sin |
| 2pz |  |  |  |  |  |  | 0 | 1 | Cos | 1 |
| 2px |  |  |  |  |  |  | 1 | 1 | Sin | Cos |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | n | normalization | exp | l | b | r | m | norm\_adj | Theta | Phi |
| 3s | 3 | 1/81sqrt(pi) | -br/3 | 0 | 3/2 | 27-18br-2(br)\*\*2 | 0 | 1/sqrt(3) | 1 | 1 |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | n | normalization | exp | l | b | r | m | norm\_adj | Theta | Phi |
| 3py | 3 |  |  | 1 | 5/2 | (6-br)r | -1 | sqrt(2) | Sin | Sin |
| 3pz | 3 |  |  | 1 |  |  | 0 | sqrt(2) | Cos | 1 |
| 3px | 3 |  |  | 1 |  |  | 1 | sqrt(2) | Sin | Cos |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | n | normalization | exp | l | b | r | m | norm\_adj | Theta | Phi |
| 3dxy | 3 |  |  | 2 | 7/2 | r\*\*2 | -2 | 1/sqrt(2) | Sin\*\*2 | Sin(2phi) |
| 3dyz | 3 |  |  | 2 |  |  | -1 | Sqrt(2) | Sin\*cos | Sin |
| 3dz2 | 3 |  |  | 2 |  |  | 0 | 1/sqrt(6) | 3cos\*\*2-1 | 1 |
| 3dxz | 3 |  |  | 2 |  |  | 1 | Sqrt(2) | Sin\*cos | Cos |
| 3dx2-y2 | 3 |  |  | 2 |  |  | 2 | 1/sqrt(2) | Sin\*\*2 | Cos(2phi) |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | n | normalization | exp | l | b | r | m | norm\_adj | Theta | Phi |
| 4s | 4 | 1/(512sqrt(pi)) | -br/4 | 0 | 3/2 | 192-144br+24(br)\*\*2-(br)\*\*3 | 0 | 1/3 | 1 | 1 |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | n | normalization | exp | l | b | r | m | norm\_adj | Theta | Phi |
| 4py | 4 |  |  | 1 | 5/2 | (80-20br+(br)\*\*2)r | -1 | 1/sqrt(5) | Sin | Sin |
| 4pz | 4 |  |  | 1 |  |  | 0 | 1/sqrt(5) | Cos | 1 |
| 4px | 4 |  |  | 1 |  |  | 1 | 1/sqrt(5) | Sin | Cos |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | n | normalization | exp | l | b | r | m | norm\_adj | Theta | Phi |
| 4dxy | 4 |  |  | 2 | 7/2 | (12-br)r\*\*2 | -2 | 1/sqrt(3) | Sin\*\*2 | Sin(2phi) |
| 4dyz | 4 |  |  | 2 |  |  | -1 | 1/sqrt(12) | Sin\*cos | sin |
| 4dz2 | 4 |  |  | 2 |  |  | 0 | 1/6 | 3cos\*\*2-1 | 1 |
| 4dxz | 4 |  |  | 2 |  |  | 1 | 1/sqrt(12) | Sin\*cos | Cos |
| 4dx2-y2 | 4 |  |  | 2 |  |  | 2 | 1/sqrt(3) | Sin\*\*2 | Cos(2phi) |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | n | normalization | exp | l | b | r | m | norm\_adj | Theta | Phi |
| 4f | 4 |  |  | 3 | 9/2 | r\*\*3 | -3 | 1/(6\*np.sqrt(2)) |  |  |
| 4f | 4 |  |  | 3 |  |  | -2 | np.sqrt(3)/(6\*np.sqrt(2)) |  |  |
| 4f | 4 |  |  | 3 |  |  | -1 | np.sqrt(3)/(6\*np.sqrt(10)) |  |  |
| 4f | 4 |  |  | 3 |  |  | 0 | 1/(6\*np.sqrt(5)) |  |  |
| 4f | 4 |  |  | 3 |  |  | 1 |  |  |  |
| 4f | 4 |  |  | 3 |  |  | 2 |  |  |  |
| 4f | 4 |  |  | 3 |  |  | 3 |  |  |  |