|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Interatomic type |  |  | Interatomic type |
| 1 | C\_C |  | 19 | O\_P |
| 2 | N\_C |  | 20 | S\_P |
| 3 | O\_C |  | 21 | C\_S |
| 4 | S\_C |  | 22 | N\_S |
| 5 | C\_N |  | 23 | O\_S |
| 6 | N\_N |  | 24 | S\_S |
| 7 | O\_N |  | 25 | C\_Cl |
| 8 | S\_N |  | 26 | N\_Cl |
| 9 | C\_O |  | 27 | O\_Cl |
| 10 | N\_O |  | 28 | S\_Cl |
| 11 | O\_O |  | 29 | C\_Br |
| 12 | S\_O |  | 30 | N\_Br |
| 13 | C\_F |  | 31 | O\_Br |
| 14 | N\_F |  | 32 | S\_Br |
| 15 | O\_F |  | 33 | C\_I |
| 16 | S\_F |  | 34 | N\_I |
| 17 | C\_P |  | 35 | O\_I |
| 18 | N\_P |  | 36 | S\_I |