SMARTS list of ionizable groups.

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|  | SMARTS | Atom\_id of  Ionization center | Acid  \_or\_  base |
| 1 | [SX4:1](=[O:2])(=[O:3])([O:4]-[C,c,N,n:5])-[OX2:6]-[H] | 6 | A |
| 2 | [SX4:1](=[O:2])(=[O:3])(-[C,c,N,n:4])-[OX2:5]-[H] | 5 | A |
| 3 | [SX3:1](=[O:2])-[O:3]-[H] | 3 | A |
| 4 | [c,n,o:1]-[C:2](=[O:3])-[O:4]-[H] | 4 | A |
| 5 | [C:1](=[O:2])-[O:3]-[H] | 3 | A |
| 6 | [C,c,N,n:1](=[O,S:2])-[SX2,OX2:3]-[H] | 3 | A |
| 7 | [c,n:1]-[SX2:2]-[H] | 2 | A |
| 8 | [C,N:1]-[SX2:2]-[H] | 2 | A |
| 9 | [PX4:1](=[O:2])(-[OX2:3]-[H])(-[O+0:4])-[OX2:5]-[H] | 3,6 | A |
| 10 | [PX4:1](=[O:2])(-[OX2:3]-[H])(-[C,c,N,n:4])-[OX2:5]-[H] | 3,6 | A |
| 11 | [PX4:1](=[O])(-[O]-[H])(-[H])-[C] | 3 | A |
| 12 | [c,n,o:1]-[O:2]-[H] | 2 | A |
| 13 | [O:1]([$(C=O),$(C[Cl]),$(CF),$(C[Br]),$(CC#N):2])-[O:3]-[H] | 3 | A |
| 14 | [C:1]-[O:2]-[O:3]-[H] | 3 | A |
| 15 | [O:1]=[C;R:2]-[C;R:3]=[C;R:4]-[O:3]-[H] | 5 | A |
| 16 | [C:1]=[C:2]-[O:3]-[H] | 3 | A |
| 17 | [C:1]-[O:2]-[H] | 2 | A |
| 18 | [C:1](=[O:2])-[N:3]-[O:4]-[H] | 4 | A |
| 19 | [O,S:1]=[C;R:2]([$([#8]),$([#7]),$([#16]),$([#6][Cl]),$([#6]F),$([#6][Br]):3])-[N;R:4]([C;R:5]=[O,S:6])-[H] | 6 | A |
| 20 | [O,S:1]=[C;R:2]-[N;R:3]([C;R:4]=[O,S:5])-[H] | 5 | A |
| 21 | [F,Cl,Br,S,s,P,p:1][#6:2][CX3:3](=[O,S:4])-[NX3+0:5]([CX3:6]=[O,S:7])-[H] | 7 | A |
| 22 | [O,S:1]=[CX3:2]-[NX3+0:3]([CX3:4]=[O,S:5])-[H] | 5 | A |
| 23 | [C:1](=[O:2])-[N:3](-[Br,Cl,I,F,S,O,N,P:4])-[H] | 4 | A |
| 24 | [C:1](=[O:2])-[N:3]-[H] | 3 | A |
| 25 | [SX4:1](=[O:2])(=[O:3])-[NX3+0:4]-[H] | 4 | A |
| 26 | [PX4:1](=[O:2])(-[C,c,N,n,F,Cl,Br,I:3])(-[C,c,N,n,F,Cl,Br,I:4])-[OX2:5]-[H] | 5 | A |
| 27 | [PX4:1](=[O:2])(-[OX2:3]-[C,c,N,n,F,Cl,Br,I:4])(-[O+0:5]-[C,c,N,n,F,Cl,Br,I:4])-[OX2:6]-[H] | 7 | A |
| 28 | [PX4:1](=[O:2])(-[OX2:3]-[C,c,N,n,F,Cl,Br,I:4])(-[C,c,N,n,F,Cl,Br,I:5])-[OX2:6]-[H] | 6 | A |
| 29 | [n:1]-[H] | 1 | A |
| 30 | [PX4:1](=[O:2])(=[O:3])(-[C,c,N,n:4])-[OX2:5]-[H] | 5 | A |
| 31 | [C:1](-[C,c:2])=[NX2:3]-[O:4]-[H] | 4 | A |
| 32 | [CX4:1]-[NX3:2](-[H])-[CX3:3](=[NX2:4])-[SH:5] | 2 | A |
| 33 | [CX3:1](=[OX1:2])-[CX4:3]-[NX3:4](-[H])-[cX3:5] | 4 | A |
| 34 | [CX3:1](=[OX1:2])-[CX4:3]-[NX3H1:4](-[H])-[CX3:5]=[NX2H0:6] | 4 | A |
| 35 | [NX3](-[H])-[C]=[C]-[C](=[O])-[C]-[O] | 1 | A |
| 36 | [c]-[NX3](-[H])-[C,n] | 2 | A |
| 37 | [NX3]-[OX2]-[H] | 2 | A |
| 38 | [SX4](=[O])(=[O])-[NX3]-[H] | 4 | A |
| 39 | [NX2]-[NX2]=[C]-[NX3]-[H] | 4 | A |
| 40 | [C]-[NX3](-[H])-[C](=[SX1]) | 2 | A |
| 41 | [C](-[C])(-[C])=[NX2]-[H] | 4 | A |
| 42 | [C]=[NX2]-[NX3](-[H])-[c] | 3 | A |
| 43 | [C]-[C](-[C,O])=[NX2]-[H] | 4 | A |
| 44 | [cX3;r6]-[NX3]-[H] | 2 | A |
| 45 | [C](=[O])-[C](-[H])(-[C])-[C](=[O]) | 3 | A |
| 46 | [PX4](=[O])(=[O])-[O]-[H] | 4 | A |
| 47 | [C](-[H])(-[C]=[O])-[C]=[O] | 1 | A |
| 48 | [C](=[S,O])-[NX3]-[H] | 3 | A |
| 49 | [S]-[S](=[O])(=[O])-[O]-[H] | 5 | A |
| 50 | [C]=[N]-[O]-[H] | 3 | A |
| 51 | [C](-[N])(=[N])-[N](-[C])-[H] | 5 | A |
| 52 | [NX2H0;r6]=[C;r6]-[C;r6](-[H])-[C]#[N] | 3 | A |
| 53 | [C]=[NX2]-[H] | 2 | A |
| 54 | [c,C]-[C](=[OX1])-[C]=[C]-[NX3]-[H] | 6 | A |
| 55 | [N:1]-[C:2](-[N:3])=[NX2:4]-[H:5] | 3 | B |
| 56 | [C:1](-[N:2])=[NX2+0:3]-[H] | 2 | B |
| 57 | [c:1]-[NX3+0:2]([H:3])[H:4] | 1 | B |
| 58 | [c:1]-[NX3+0:2]([H:3])[!H:4] | 1 | B |
| 59 | [c:1]-[NX3+1:2]([!H:3])([!H:4])-[H] | 1 | B |
| 60 | [n+1&H1:1] | 0 | B |
| 61 | [C:1]-[NX4+1:2]-[H] | 1 | B |
| 62 | [C,c:1]-[O:2]-[NH2:3] | 2 | B |
| 63 | [CX4:1]-[NX3:2]([CX4,c:3])([CX4,c:4]) | 1 | B |
| 64 | [C:1](-[C,c:2])=[NX2:3]-[O:4]-[H] | 2 | B |
| 65 | [C:1]-[nX3;H0:2]([C,c:3])([C,c:4]) | 1 | B |
| 66 | [c:1]:[nX2:2]:[c:3] | 1 | B |
| 67 | [c:1]:[nX2:2]:[nX3:3]:[c:4]=[OX1:5] | 1 | B |
| 68 | [CX4:1]-[NX3:2](-[H])-[CX4:3] | 1 | B |
| 69 | [C:1](=[O:2])-[N:3](-[H])-[NX3:4](-[H])(-[H]) | 4 | B |
| 70 | [c:1]:[nX2:2]:[n:3]:[n:4]:[n:5]-[CX4:6] | 1 | B |
| 71 | [CX4:1](-[CX4])(-[CX4])-[NH2:2] | 3 | B |
| 72 | [CX3:1]=[NX2:2]-[CX4,SX4:3] | 1 | B |
| 73 | [c:1]-[NH2] | 1 | B |
| 74 | [!OX1][C,c:1]-[NX3:2](-[c:3])-[H] | 2 | B |
| 75 | [C,c:1]-[NX2:2]=[c:3]:[nX3:4]-[H] | 1 | B |
| 76 | [nX2:1](:[c:2]):[nX3:3]-[c:4] | 0 | B |
| 77 | [c:1]=[NX2:2]-[H] | 1 | B |
| 78 | [c:1]:[nX2:2]:[nX2:3]:[nX3](-[H]):[nX2:4] | 1 | B |
| 79 | [OX1:1]=[CX3:2]-[C:3]-[NH2:4] | 3 | B |
| 80 | [C:1]=[N:2]-[N:3]=[C:4](-[NH2:5])-[S,O,P:6] | 2 | B |
| 81 | [nH1:1]:[c:2]:[nX2H0:3]:[nX2H0:4]:[cX3:5]:[cX3:6] | 2,3 | B |
| 83 | [cX3:1]:[nX2H0:2]:[nX2H0:3]:[cX3:4]:[sX2H0:5] | 1,2 | B |
| 84 | [cX3:1]:[cX3:2]:[nX2H0:3]:[nX2H0:4]:[cX3:5]:[cX3:6]:[cX3:7]:[nX3:8]:[cX3:9] | 2,3 | B |
| 85 | [NX3H0:1]-[CX3:2]=[NX2H0:3]-[NX2H0:4]=[CX3:5] | 2 | B |
| 86 | [CX3:1]=[NX2H0:2]-[NX3H1:3]-[CX4:4] | 1,2 | B |
| 87 | [CX3:1](=[OX1:2])-[CX4:3]-[NX3:4](-[H])-[cX3:5] | 3 | B |
| 88 | [CX3:1](=[OX1:2])-[CX4:3]-[NX3H1:4](-[H])-[CX3:5]=[NX2H0:6] | 6 | B |
| 89 | [C:1]-[NH:2]-[NH:3]-[C:4]=[O:5] | 1 | B |
| 90 | [C:1]=[NX2:2]-[OX2:3] | 1 | B |
| 91 | [PX4:1](=[OX1:2])(-[NH2:3])(-[NH1:4]) | 2,3 | B |
| 92 | [c:1]:[nX2H0:2]:[nX2H0:3]:[cX3:4]:[nX3:5]-[NX3] | 1,2 | B |
| 93 | [c:1]:[nX2:2]:[nX3:3]:[cX3:4]:[cX3:5] | 1 | B |
| 94 | [C]=[NX2]-[C] | 1 | B |
| 95 | [PX4:1](-[NH1:2])=[OX1:3] | 1 | B |
| 96 | [CX4:1]-[CX4:2]-[NH2:3] | 2 | B |
| 97 | [c:1]=[NX2] | 1 | B |
| 98 | [PX4]-[NX3H0] | 1 | B |
| 99 | [C:1]-[NX3:2]-[C:3](=[SX1])-[NX3:4]-[C:5] | 3 | B |
| 100 | [OX2]-[C](=[OX1])-[NX3]-[NX3] | 4 | B |
| 101 | [c]-[NX2]=[C] | 1 | B |
| 102 | [c,S]-[C]-[NH2] | 2 | B |
| 103 | [NX3]-[OX2]-[H] | 0 | B |
| 104 | [c]:[n]:[n]:[c]:[nX3]-[c] | 1,2 | B |
| 105 | [C]-[C]-[NH2] | 2 | B |
| 106 | [S]-[NH1]-[C] | 1 | B |
| 107 | [c]-[NX3](-[H])-[c] | 1 | B |
| 108 | [C]=[NX2]-[NX2]=[C]-[NH2] | 2 | B |
| 109 | [C]-[C]-[C]=[NX2H0]-[NX3H0] | 3,4 | B |
| 110 | [c]-[NX3H1]-[C]-[C]=[C]-[c] | 1 | B |
| 111 | [NX3]-[C](=[S])-[NX3] | 2 | B |
| 112 | [c]:[nH0]:[nH0]:[c]:[c]:[c] | 1,2 | B |
| 113 | [c]:[c]-[nX3H1]-[C]-[C]=[C] | 2 | B |
| 114 | [C]=[C]-[NX3H0](-[C]-[C])(-[C]-[C]) | 2 | B |
| 115 | [nX3]:[c]:[nX2]:[nX2]:[c] | 2,3 | B |
| 116 | [n]-[NX3H2] | 1 | B |
| 117 | [nX3H1]:[c]:[c]:[c](=[O]):[c]:[c] | 4 | B |
| 118 | [C]-[NX3H1]-[NX3H2] | 1,2 | B |
| 119 | [OX2]-[C]-[NX3H2] | 2 | B |
| 120 | [c]:[nX2H0]:[nX2H0]:[nX3H0]:[c] | 1 | B |
| 121 | [SX4](=[O])(=[O])-[NX3H2] | 3 | B |
| 122 | [NX3H0](-[C;!CSX1])(-[C;!CSX1])-[C;!CSX1] | 0 | B |
| 123 | [c]:[c]:[c]:[c](-[OH]):[nX3H1] | 5 | B |
| 124 | [C]-[C]-[NX3H0]-[OX2]-[C] | 2 | B |
| 125 | [c]:[c]-[NX3H1]-[C]-[C]-[C]-[c] | 2 | B |
| 126 | [C](=[NX2H1])(-[C])-[C] | 1 | B |
| 127 | [C,c]-[NX2H0]=[NX2H0]-[NX3] | 3 | B |
| 128 | [c]:[c]:[c]:[c]:[nX3]-[cX3] | 4 | B |
| 129 | [nX2H0]:[nX2H0]:[nX2H0]:[nX3H0]:[c]:[c] | 0 | B |
| 130 | [C]=[NX2]-[NH1]-[c] | 1 | B |
| 131 | [C]-[C](-[C,O])=[NH1] | 3 | B |
| 132 | [C]-[NX3H0](-[C])-[NX3H1]-[C] | 1 | B |
| 133 | [nX2]:[nX2]:[cX3](-[C]):[nX2]:[nX3]-[C] | 1 | B |
| 134 | [c]-[C]=[NX2H0]-[NX2H0]=[C]-[SH] | 3 | B |
| 135 | [c]-[c]:[nX2H0]:[nX2H0]:[nX3](-[C]):[nX2] | 2 | B |
| 136 | [c](=[SX1]):[nX3H1]:[c] | 1,2 | B |
| 137 | [C]=[NX2H0]-[NX3H0](-[C])-[C] | 1,2 | B |
| 138 | [c]:[nX2H0]:[sX2H0]:[c]:[c] | 1 | B |
| 139 | [C]=[NX2H0]-[NH2] | 1,2 | B |
| 140 | [nX2H0]:[nX2H0]:[c]:[nH1]:[c]:[c]:[c] | 1 | B |
| 141 | [NX2H0;r7]-[NX2H0;r7]=[C;r7]-[NH1;r7]-[c;r7]:[c;r7]-[C;r7] | 1 | B |
| 142 | [NX3](-[C])(-[C])-[C]=[S] | 0 | B |
| 143 | [c]:[nX2H0]:[nX2H0]:[nX2H0]:[nX3H0] | 1 | B |
| 144 | [c;r5]:[c;r5]:[c;r5]:[c;r5]:[nH1;r5] | 4 | B |