**Separation of heterocyclic nitrogen compounds from coal tar fractions *via* ionic liquids: COSMO-SAC screening and experimental study**

*Dongmei Xu a, Mi Zhang a, Jun Gao a,, Lianzheng Zhang a,\*, Shixue Zhou a,Yinglong Wang b*

a College of Chemical and Environmental Engineering, Shandong University of Science and Technology, Qingdao 266590, China

b College of Chemical and Engineering, Qingdao University of Science and Technology, Qingdao, 266042, China

\*Corresponding author

Lianzheng Zhang, E-mail address: zhanglz@sdust.edu.cn, Tel: +86-532-86057799.

Table S1. The geometry optimization INPUT file for DMo13 module

|  |
| --- |
| # The parameters of geometry optimization |
| # Task parameters  Calculate optimize  Opt\_energy\_convergence 1.0000e-005  Opt\_gradient\_convergence 2.0000e-003 A  Opt\_displacement\_convergence 5.0000e-003 A  Opt\_iterations 200  Opt\_max\_displacement 0.3000 A  Initial\_hessian improved  Symmetry on  Max\_memory 4096  File\_usage smart  # Electronic parameters  Spin\_polarization restricted  Charge 0  Basis dnp  basis\_version basfile\_v4.4  Pseudopotential none  Functional vwn-bp  Aux\_density octupole  Integration\_grid fine  Occupation thermal 0.0050  Cutoff\_Global 5.5000 angstrom  Scf\_density\_convergence 1.0000e-006  Scf\_charge\_mixing 2.0000e-001  Scf\_iterations 200  Scf\_diis 6 pulay  # Print options  Print eigval\_last\_it |

Table S2. The COSMO calculation INPUT file for DMo13 module

|  |
| --- |
| # The parameters of geometry optimization |
| # Task parameters  Calculate energy  Symmetry on  Max\_memory 4096  File\_usage smart  # Electronic parameters  Spin\_polarization restricted  Charge 0  Basis dnp  Pseudopotential none  Functional vwn-bp  Aux\_density octupole  Integration\_grid fine  Occupation thermal 0.0050  Cutoff\_Global 5.5000 angstrom  Scf\_density\_convergence 1.0000e-006  Scf\_charge\_mixing 2.0000e-001  Scf\_iterations 50  Scf\_diis 6 pulay  basis\_version v4.0.0  # COSMO Environment Keywords  Cosmo on  Cosmo\_Grid\_Size 1082  Cosmo\_Segments 92  Cosmo\_Solvent\_Radius 1.300000  Cosmo\_A-Matrix\_Cutoff 7.000000  Cosmo\_Radius\_Incr 0.000000  Cosmo\_A-Constant 1.882190  Cosmo\_B-Constant 0.010140  Cosmo\_RadCorr\_Incr 0.150000  Cosmo\_Atomic\_Radii  1 1.300000  3 1.570000  5 2.048000  6 2.000000  7 1.830000  8 1.720000  9 1.720000  11 1.800000  14 2.200000  15 2.120000  16 2.160000  17 2.050000  19 2.223000  30 1.626000  32 2.700000  33 2.350000  34 2.200000  35 2.160000  50 2.550000  53 2.320000  # Print options  Print eigval\_last\_it  # Calculated properties |

Table S3. The cavity volume and surface area parameters of cations and anions adopted from the COSMO calculation

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| No. | Cations and Anions | Total number of segments | Surface area of cavity/ A2 | Total Volume of cavity/ A3 |
| **Anions** | | | | |
| 1 | Cl- | 92 | 52.810173 | 36.086951 |
| 2 | Br- | 92 | 58.629659 | 42.213354 |
| 3 | I- | 92 | 67.637233 | 52.306127 |
| 4 | Ac- | 340 | 90.350767 | 72.521813 |
| 5 | Pro- | 442 | 109.013702 | 93.851412 |
| 6 | TA- | 370 | 112.923099 | 98.608158 |
| 7 | Tos- | 755 | 185.948127 | 186.547645 |
| 8 | OTf- | 406 | 126.425855 | 117.134920 |
| 9 | MeSO4- | 423 | 116.461312 | 102.563912 |
| 10 | EtSO4- | 532 | 136.441266 | 123.422578 |
| 11 | CH3OEtSO4- | 681 | 168.956785 | 157.619450 |
| 12 | PFBS- | 636 | 203.190521 | 228.443303 |
| 13 | HSO4- | 329 | 96.933787 | 79.791199 |
| 14 | H2PO4- | 350 | 101.406923 | 84.477958 |
| 15 | Me2PO4- | 574 | 141.663691 | 130.588543 |
| 16 | FAP- | 788 | 255.977255 | 320.396580 |
| 17 | PF6- | 342 | 114.288490 | 103.361412 |
| 18 | BF4- | 298 | 91.107606 | 73.326292 |
| 19 | TCB- | 484 | 161.430491 | 148.601338 |
| 20 | SbF6- | 372 | 131.258926 | 123.135221 |
| 21 | ClO4- | 298 | 93.928496 | 76.018119 |
| 22 | NO3- | 240 | 76.525165 | 56.893976 |
| 23 | AlCl4- | 313 | 155.440598 | 160.234117 |
| 24 | FeCl4- | 344 | 153.521068 | 149.208121 |
| 25 | SCN- | 207 | 86.705355 | 69.483466 |
| 26 | TCM- | 398 | 131.666423 | 114.014422 |
| 27 | DCA- | 298 | 102.256764 | 82.999843 |
| 28 | NTf2 | 606 | 197.369077 | 214.948176 |
| 29 | PhO- | 559 | 129.747536 | 119.268506 |
| **Cations** | | | | |
| 1 | Mmim+ | 605 | 143.732619 | 133.745918 |
| 2 | Emim+ | 698 | 162.286341 | 156.228718 |
| 3 | Pmim+ | 809 | 182.438644 | 178.210781 |
| 4 | Bmim+ | 895 | 200.853661 | 201.015361 |
| 5 | Pnmim+ | 1027 | 222.275991 | 222.129829 |
| 6 | Hmim+ | 1129 | 241.834637 | 243.426429 |
| 7 | Omim+ | 1340 | 281.788167 | 287.502028 |
| 8 | Dmim+ | 1561 | 321.565764 | 330.831937 |
| 9 | C12-mim+ | 1772 | 361.408686 | 374.813225 |
| 10 | C14-mim+ | 1991 | 400.358229 | 416.705481 |
| 11 | C16-mim+ | 2207 | 439.892890 | 459.896795 |
| 12 | Amim+ | 742 | 176.994745 | 172.452470 |
| 13 | Bnmim+ | 985 | 220.437009 | 228.982016 |
| 14 | HOemim+ | 740 | 173.692939 | 168.009801 |
| 15 | CPmim+ | 870 | 207.040688 | 204.793296 |
| 16 | C3NH2mim+ | 875 | 197.418732 | 194.165639 |
| 17 | EOOEmim+ | 939 | 215.691072 | 212.599384 |
| 18 | MOEmim+ | 845 | 194.946274 | 190.205528 |
| 19 | HO2Mmim+ | 711 | 174.087254 | 169.869832 |
| 20 | HO2Etmim+ | 823 | 196.954508 | 194.609325 |
| 21 | PrSO3Hmim+ | 987 | 231.610160 | 235.421928 |
| 22 | EPy+ | 682 | 155.399980 | 149.378021 |
| 23 | BPy+ | 894 | 194.817672 | 192.952243 |
| 24 | BmPy+ | 998 | 213.697169 | 213.857279 |
| 25 | HPy+ | 1114 | 234.841569 | 236.984327 |
| 26 | OPy+ | 1320 | 274.615259 | 280.849135 |
| 27 | PrSO3HPy+ | 959 | 223.738668 | 228.672203 |
| 28 | N1111+ | 468 | 112.396441 | 98.033946 |
| 29 | N1222+ | 758 | 172.165617 | 183.752668 |
| 30 | N122,1O2+ | 908 | 204.694972 | 218.178034 |
| 31 | N1444+ | 1346 | 289.379418 | 315.721219 |
| 32 | P1444+ | 1506 | 309.095854 | 334.165993 |
| 33 | P2444+ | 1481 | 312.545211 | 352.979734 |
| 34 | P4444+ | 1677 | 349.285740 | 394.509728 |
| 35 | P4446+ | 1885 | 389.114266 | 438.128457 |
| 36 | P14+ | 934 | 204.165743 | 215.159434 |
| 37 | PP14+ | 1027 | 215.160885 | 231.543531 |
| 38 | BmMor+ | 968 | 209.749314 | 223.711216 |
| 39 | Tmgh+ | 731 | 166.863724 | 172.846961 |

Table S4. The *σ*-profile of different cations and anions.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Cations | | | | | |
| Mmim+ |  | Emim+ |  | Pmim+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.244676 | -0.015 | 0.334466 | -0.015 | 0.210066 |
| -0.014 | 2.649317 | -0.014 | 2.606394 | -0.014 | 2.506000 |
| -0.013 | 3.237749 | -0.013 | 2.587532 | -0.013 | 2.853866 |
| -0.012 | 4.153271 | -0.012 | 4.257409 | -0.012 | 4.355001 |
| -0.011 | 9.120567 | -0.011 | 8.117550 | -0.011 | 8.027790 |
| -0.010 | 8.001797 | -0.010 | 8.422996 | -0.010 | 7.710602 |
| -0.009 | 16.235460 | -0.009 | 15.175377 | -0.009 | 14.029542 |
| -0.008 | 19.814273 | -0.008 | 15.329022 | -0.008 | 15.400341 |
| -0.007 | 15.902683 | -0.007 | 14.705261 | -0.007 | 13.497403 |
| -0.006 | 16.332795 | -0.006 | 18.424431 | -0.006 | 16.278484 |
| -0.005 | 24.268838 | -0.005 | 24.209001 | -0.005 | 24.122271 |
| -0.004 | 8.563698 | -0.004 | 15.729690 | -0.004 | 20.751389 |
| -0.003 | 3.726944 | -0.003 | 7.400752 | -0.003 | 13.336315 |
| -0.002 | 3.164480 | -0.002 | 8.740005 | -0.002 | 11.542862 |
| -0.001 | 3.334980 | -0.001 | 8.405743 | -0.001 | 11.051886 |
| 0.000 | 2.571573 | 0.000 | 5.238711 | 0.000 | 7.469424 |
| 0.001 | 2.409538 | 0.001 | 2.602024 | 0.001 | 8.285330 |
| 0.002 | 0.000000 | 0.002 | 0.000000 | 0.002 | 1.010098 |
| 0.003 | 0.000000 | 0.003 | 0.000000 | 0.003 | 0.000000 |
| 0.004 | 0.000000 | 0.004 | 0.000000 | 0.004 | 0.000000 |
| 0.005 | 0.000000 | 0.005 | 0.000000 | 0.005 | 0.000000 |
| 0.006 | 0.000000 | 0.006 | 0.000000 | 0.006 | 0.000000 |
| 0.007 | 0.000000 | 0.007 | 0.000000 | 0.007 | 0.000000 |
| 0.008 | 0.000000 | 0.008 | 0.000000 | 0.008 | 0.000000 |
| 0.009 | 0.000000 | 0.009 | 0.000000 | 0.009 | 0.000000 |
| 0.010 | 0.000000 | 0.010 | 0.000000 | 0.010 | 0.000000 |
| 0.011 | 0.000000 | 0.011 | 0.000000 | 0.011 | 0.000000 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 0.000000 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| Bmim+ |  | Pnmim+ |  | Hmim+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.116493 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.666395 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 1.656107 | -0.015 | 0.221752 | -0.015 | 0.235364 |
| -0.014 | 1.158264 | -0.014 | 2.314791 | -0.014 | 2.462306 |
| -0.013 | 7.722734 | -0.013 | 2.844952 | -0.013 | 2.919049 |
| -0.012 | 7.013346 | -0.012 | 4.442939 | -0.012 | 4.321246 |
| -0.011 | 6.165825 | -0.011 | 7.907917 | -0.011 | 7.792603 |
| -0.010 | 7.052865 | -0.010 | 8.046293 | -0.010 | 7.916981 |
| -0.009 | 10.800061 | -0.009 | 13.879261 | -0.009 | 14.044776 |
| -0.008 | 14.997614 | -0.008 | 15.792144 | -0.008 | 15.529529 |
| -0.007 | 13.513325 | -0.007 | 12.399401 | -0.007 | 12.572102 |
| -0.006 | 14.593576 | -0.006 | 16.320141 | -0.006 | 16.041957 |
| -0.005 | 16.731900 | -0.005 | 21.738716 | -0.005 | 22.256150 |
| -0.004 | 17.080448 | -0.004 | 18.842635 | -0.004 | 17.887821 |
| -0.003 | 19.350397 | -0.003 | 21.409502 | -0.003 | 21.672643 |
| -0.002 | 17.500619 | -0.002 | 21.057748 | -0.002 | 25.863495 |
| -0.001 | 12.937403 | -0.001 | 19.077905 | -0.001 | 24.612977 |
| 0.000 | 11.650055 | 0.000 | 13.233979 | 0.000 | 16.913751 |
| 0.001 | 9.979057 | 0.001 | 11.553848 | 0.001 | 13.500229 |
| 0.002 | 8.239935 | 0.002 | 9.459228 | 0.002 | 11.620938 |
| 0.003 | 1.762915 | 0.003 | 1.724633 | 0.003 | 3.559991 |
| 0.004 | 0.164356 | 0.004 | 0.008239 | 0.004 | 0.110763 |
| 0.005 | 0.000000 | 0.005 | 0.000000 | 0.005 | 0.000000 |
| 0.006 | 0.000000 | 0.006 | 0.000000 | 0.006 | 0.000000 |
| 0.007 | 0.000000 | 0.007 | 0.000000 | 0.007 | 0.000000 |
| 0.008 | 0.000000 | 0.008 | 0.000000 | 0.008 | 0.000000 |
| 0.009 | 0.000000 | 0.009 | 0.000000 | 0.009 | 0.000000 |
| 0.010 | 0.000000 | 0.010 | 0.000000 | 0.010 | 0.000000 |
| 0.011 | 0.000000 | 0.011 | 0.000000 | 0.011 | 0.000000 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 0.000000 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| Omim+ |  | Dmim+ |  | C12mim+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.209416 | -0.015 | 0.220976 | -0.015 | 0.212431 |
| -0.014 | 2.473240 | -0.014 | 2.301250 | -0.014 | 2.532819 |
| -0.013 | 2.743130 | -0.013 | 2.947055 | -0.013 | 2.777398 |
| -0.012 | 4.329754 | -0.012 | 4.349136 | -0.012 | 4.550271 |
| -0.011 | 7.775857 | -0.011 | 7.837862 | -0.011 | 7.878839 |
| -0.010 | 7.877066 | -0.010 | 7.784178 | -0.010 | 7.611427 |
| -0.009 | 14.116279 | -0.009 | 13.955500 | -0.009 | 13.341822 |
| -0.008 | 15.593107 | -0.008 | 15.484711 | -0.008 | 16.342721 |
| -0.007 | 12.738898 | -0.007 | 13.241396 | -0.007 | 12.985574 |
| -0.006 | 16.285562 | -0.006 | 16.402001 | -0.006 | 16.180104 |
| -0.005 | 21.900704 | -0.005 | 21.514547 | -0.005 | 21.328471 |
| -0.004 | 17.878608 | -0.004 | 17.869273 | -0.004 | 18.183352 |
| -0.003 | 21.866203 | -0.003 | 22.632031 | -0.003 | 23.217249 |
| -0.002 | 33.959305 | -0.002 | 40.472292 | -0.002 | 47.158193 |
| -0.001 | 34.203980 | -0.001 | 44.385389 | -0.001 | 54.621058 |
| 0.000 | 26.341393 | 0.000 | 35.176549 | 0.000 | 44.033018 |
| 0.001 | 18.846846 | 0.001 | 25.235833 | 0.001 | 31.725087 |
| 0.002 | 14.926492 | 0.002 | 18.029083 | 0.002 | 21.015017 |
| 0.003 | 7.496366 | 0.003 | 11.508393 | 0.003 | 15.456334 |
| 0.004 | 0.226001 | 0.004 | 0.218357 | 0.004 | 0.257552 |
| 0.005 | 0.000000 | 0.005 | 0.000000 | 0.005 | 0.000000 |
| 0.006 | 0.000000 | 0.006 | 0.000000 | 0.006 | 0.000000 |
| 0.007 | 0.000000 | 0.007 | 0.000000 | 0.007 | 0.000000 |
| 0.008 | 0.000000 | 0.008 | 0.000000 | 0.008 | 0.000000 |
| 0.009 | 0.000000 | 0.009 | 0.000000 | 0.009 | 0.000000 |
| 0.010 | 0.000000 | 0.010 | 0.000000 | 0.010 | 0.000000 |
| 0.011 | 0.000000 | 0.011 | 0.000000 | 0.011 | 0.000000 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 0.000000 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| C14mim+ |  | C16mim+ |  | BmPy+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.129490 | -0.015 | 0.151373 | -0.015 | 0.000000 |
| -0.014 | 2.199788 | -0.014 | 2.340561 | -0.014 | 0.000000 |
| -0.013 | 2.441479 | -0.013 | 2.496375 | -0.013 | 0.417525 |
| -0.012 | 3.762859 | -0.012 | 3.754207 | -0.012 | 4.012399 |
| -0.011 | 5.695877 | -0.011 | 6.302431 | -0.011 | 4.578139 |
| -0.010 | 7.003093 | -0.010 | 6.705605 | -0.010 | 11.050673 |
| -0.009 | 13.702300 | -0.009 | 13.331050 | -0.009 | 13.773007 |
| -0.008 | 19.087649 | -0.008 | 18.253807 | -0.008 | 13.462606 |
| -0.007 | 13.738131 | -0.007 | 13.739873 | -0.007 | 18.273228 |
| -0.006 | 20.421929 | -0.006 | 20.866663 | -0.006 | 16.962384 |
| -0.005 | 20.261791 | -0.005 | 21.273567 | -0.005 | 21.701800 |
| -0.004 | 19.357432 | -0.004 | 18.526532 | -0.004 | 22.906424 |
| -0.003 | 22.365611 | -0.003 | 23.313654 | -0.003 | 25.767131 |
| -0.002 | 54.050507 | -0.002 | 60.248195 | -0.002 | 25.550473 |
| -0.001 | 62.901618 | -0.001 | 73.034807 | -0.001 | 14.751126 |
| 0.000 | 50.923286 | 0.000 | 59.850229 | 0.000 | 8.759319 |
| 0.001 | 39.048568 | 0.001 | 45.289220 | 0.001 | 6.681990 |
| 0.002 | 23.866458 | 0.002 | 26.738596 | 0.002 | 4.490605 |
| 0.003 | 19.103536 | 0.003 | 23.204350 | 0.003 | 0.558370 |
| 0.004 | 0.296882 | 0.004 | 0.471857 | 0.004 | 0.000000 |
| 0.005 | 0.000000 | 0.005 | 0.000000 | 0.005 | 0.000000 |
| 0.006 | 0.000000 | 0.006 | 0.000000 | 0.006 | 0.000000 |
| 0.007 | 0.000000 | 0.007 | 0.000000 | 0.007 | 0.000000 |
| 0.008 | 0.000000 | 0.008 | 0.000000 | 0.008 | 0.000000 |
| 0.009 | 0.000000 | 0.009 | 0.000000 | 0.009 | 0.000000 |
| 0.010 | 0.000000 | 0.010 | 0.000000 | 0.010 | 0.000000 |
| 0.011 | 0.000000 | 0.011 | 0.000000 | 0.011 | 0.000000 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 0.000000 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| N1444+ |  | P1444+ |  | P14+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 0.000000 |
| -0.012 | 0.000000 | -0.012 | 0.000000 | -0.012 | 0.000000 |
| -0.011 | 1.408241 | -0.011 | 0.112213 | -0.011 | 0.996371 |
| -0.010 | 8.185596 | -0.010 | 5.774746 | -0.010 | 10.216654 |
| -0.009 | 16.595242 | -0.009 | 15.590544 | -0.009 | 19.031601 |
| -0.008 | 13.730313 | -0.008 | 16.696763 | -0.008 | 16.530915 |
| -0.007 | 15.657025 | -0.007 | 16.598401 | -0.007 | 19.850375 |
| -0.006 | 21.864295 | -0.006 | 21.460509 | -0.006 | 29.006503 |
| -0.005 | 24.411269 | -0.005 | 23.075188 | -0.005 | 24.405040 |
| -0.004 | 33.430718 | -0.004 | 36.309852 | -0.004 | 18.255286 |
| -0.003 | 37.175554 | -0.003 | 42.406650 | -0.003 | 16.986138 |
| -0.002 | 35.866119 | -0.002 | 39.164817 | -0.002 | 18.044899 |
| -0.001 | 22.283443 | -0.001 | 25.170765 | -0.001 | 10.332649 |
| 0.000 | 23.404183 | 0.000 | 25.698432 | 0.000 | 8.063088 |
| 0.001 | 19.849968 | 0.001 | 21.512791 | 0.001 | 6.899225 |
| 0.002 | 13.748257 | 0.002 | 17.249168 | 0.002 | 4.919007 |
| 0.003 | 1.769238 | 0.003 | 2.275058 | 0.003 | 0.628021 |
| 0.004 | 0.000000 | 0.004 | 0.000000 | 0.004 | 0.000000 |
| 0.005 | 0.000000 | 0.005 | 0.000000 | 0.005 | 0.000000 |
| 0.006 | 0.000000 | 0.006 | 0.000000 | 0.006 | 0.000000 |
| 0.007 | 0.000000 | 0.007 | 0.000000 | 0.007 | 0.000000 |
| 0.008 | 0.000000 | 0.008 | 0.000000 | 0.008 | 0.000000 |
| 0.009 | 0.000000 | 0.009 | 0.000000 | 0.009 | 0.000000 |
| 0.010 | 0.000000 | 0.010 | 0.000000 | 0.010 | 0.000000 |
| 0.011 | 0.000000 | 0.011 | 0.000000 | 0.011 | 0.000000 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 0.000000 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| PP14+ |  | BmMor+ |  | Amim+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.400204 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 2.916671 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 2.938343 |
| -0.012 | 0.000000 | -0.012 | 0.496344 | -0.012 | 3.454612 |
| -0.011 | 1.486682 | -0.011 | 8.521287 | -0.011 | 8.512921 |
| -0.010 | 9.165823 | -0.010 | 17.358999 | -0.010 | 7.827694 |
| -0.009 | 17.885049 | -0.009 | 19.010706 | -0.009 | 14.406226 |
| -0.008 | 15.897626 | -0.008 | 24.536276 | -0.008 | 19.695909 |
| -0.007 | 17.108308 | -0.007 | 21.946834 | -0.007 | 19.527087 |
| -0.006 | 26.804217 | -0.006 | 19.246437 | -0.006 | 19.265954 |
| -0.005 | 26.277161 | -0.005 | 13.144226 | -0.005 | 21.960120 |
| -0.004 | 24.662564 | -0.004 | 14.503317 | -0.004 | 10.799141 |
| -0.003 | 20.382068 | -0.003 | 14.191695 | -0.003 | 7.694455 |
| -0.002 | 20.896899 | -0.002 | 13.808078 | -0.002 | 8.521134 |
| -0.001 | 12.636966 | -0.001 | 8.690646 | -0.001 | 7.623221 |
| 0.000 | 9.836347 | 0.000 | 8.999507 | 0.000 | 5.996474 |
| 0.001 | 6.683524 | 0.001 | 7.778659 | 0.001 | 6.018948 |
| 0.002 | 4.815255 | 0.002 | 5.186537 | 0.002 | 3.263637 |
| 0.003 | 0.622428 | 0.003 | 1.545443 | 0.003 | 2.335048 |
| 0.004 | 0.000000 | 0.004 | 1.427566 | 0.004 | 1.763759 |
| 0.005 | 0.000000 | 0.005 | 0.953602 | 0.005 | 1.297484 |
| 0.006 | 0.000000 | 0.006 | 0.748286 | 0.006 | 0.756071 |
| 0.007 | 0.000000 | 0.007 | 1.384063 | 0.007 | 0.019658 |
| 0.008 | 0.000000 | 0.008 | 1.000781 | 0.008 | 0.000000 |
| 0.009 | 0.000000 | 0.009 | 1.607424 | 0.009 | 0.000000 |
| 0.010 | 0.000000 | 0.010 | 1.531805 | 0.010 | 0.000000 |
| 0.011 | 0.000000 | 0.011 | 1.673535 | 0.011 | 0.000000 |
| 0.012 | 0.000000 | 0.012 | 0.457291 | 0.012 | 0.000000 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| Bnmim+ |  | C3NH2mim+ |  | CPmim+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.634950 | -0.015 | 0.403616 | -0.015 | 0.700201 |
| -0.014 | 2.712896 | -0.014 | 2.509739 | -0.014 | 3.014266 |
| -0.013 | 2.383364 | -0.013 | 2.750947 | -0.013 | 3.157057 |
| -0.012 | 3.493948 | -0.012 | 4.317089 | -0.012 | 5.352337 |
| -0.011 | 5.737062 | -0.011 | 8.869660 | -0.011 | 10.361095 |
| -0.010 | 9.611084 | -0.010 | 10.759853 | -0.010 | 15.740796 |
| -0.009 | 18.933322 | -0.009 | 17.232421 | -0.009 | 24.092291 |
| -0.008 | 17.689404 | -0.008 | 17.671583 | -0.008 | 25.585913 |
| -0.007 | 19.775706 | -0.007 | 15.824273 | -0.007 | 19.185194 |
| -0.006 | 22.965979 | -0.006 | 19.869621 | -0.006 | 17.073943 |
| -0.005 | 26.692862 | -0.005 | 28.412488 | -0.005 | 19.923920 |
| -0.004 | 12.413720 | -0.004 | 17.971205 | -0.004 | 8.469578 |
| -0.003 | 11.428126 | -0.003 | 11.003332 | -0.003 | 5.444669 |
| -0.002 | 10.623042 | -0.002 | 9.497103 | -0.002 | 6.866512 |
| -0.001 | 8.486747 | -0.001 | 7.460114 | -0.001 | 3.387411 |
| 0.000 | 9.331538 | 0.000 | 6.214533 | 0.000 | 4.072206 |
| 0.001 | 7.909967 | 0.001 | 3.802112 | 0.001 | 3.793221 |
| 0.002 | 6.409662 | 0.002 | 1.091820 | 0.002 | 2.573437 |
| 0.003 | 7.952156 | 0.003 | 1.296437 | 0.003 | 1.007379 |
| 0.004 | 8.569996 | 0.004 | 0.604495 | 0.004 | 1.357454 |
| 0.005 | 5.398278 | 0.005 | 0.593424 | 0.005 | 1.472065 |
| 0.006 | 1.283234 | 0.006 | 0.822988 | 0.006 | 1.775394 |
| 0.007 | 0.000000 | 0.007 | 0.846813 | 0.007 | 2.221269 |
| 0.008 | 0.000000 | 0.008 | 0.985512 | 0.008 | 3.829098 |
| 0.009 | 0.000000 | 0.009 | 0.786329 | 0.009 | 4.020301 |
| 0.010 | 0.000000 | 0.010 | 0.672639 | 0.010 | 5.444061 |
| 0.011 | 0.000000 | 0.011 | 0.015311 | 0.011 | 4.165234 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 2.748807 |
| 0.013 | 0.000000 | 0.013 | 0.707475 | 0.013 | 0.205587 |
| 0.014 | 0.000000 | 0.014 | 0.763454 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 1.466012 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.251652 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.612136 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.462205 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.818096 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.052274 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| EOOEmim+ | | HO2CEtmim+ |  | HO2Cmmim+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.067595 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.674571 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 1.577530 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.866139 |
| -0.019 | 0.000000 | -0.019 | 0.515858 | -0.019 | 0.377174 |
| -0.018 | 0.000000 | -0.018 | 1.311441 | -0.018 | 0.778080 |
| -0.017 | 0.000000 | -0.017 | 0.325910 | -0.017 | 2.220330 |
| -0.016 | 0.000000 | -0.016 | 1.231473 | -0.016 | 1.489184 |
| -0.015 | 0.000000 | -0.015 | 2.410857 | -0.015 | 0.915168 |
| -0.014 | 0.901730 | -0.014 | 4.102549 | -0.014 | 5.329012 |
| -0.013 | 3.740438 | -0.013 | 3.117635 | -0.013 | 10.798323 |
| -0.012 | 9.928540 | -0.012 | 5.830315 | -0.012 | 10.077783 |
| -0.011 | 12.649370 | -0.011 | 10.715298 | -0.011 | 10.298254 |
| -0.010 | 8.905276 | -0.010 | 11.973003 | -0.010 | 7.901039 |
| -0.009 | 12.976661 | -0.009 | 19.946157 | -0.009 | 13.213286 |
| -0.008 | 14.996910 | -0.008 | 18.411273 | -0.008 | 13.337120 |
| -0.007 | 15.755688 | -0.007 | 14.955340 | -0.007 | 10.061227 |
| -0.006 | 18.549461 | -0.006 | 14.892464 | -0.006 | 12.563366 |
| -0.005 | 24.914303 | -0.005 | 21.485560 | -0.005 | 15.079896 |
| -0.004 | 17.529489 | -0.004 | 10.075436 | -0.004 | 6.605911 |
| -0.003 | 15.446846 | -0.003 | 7.323599 | -0.003 | 4.852794 |
| -0.002 | 11.078010 | -0.002 | 6.219101 | -0.002 | 4.348562 |
| -0.001 | 9.684171 | -0.001 | 4.885452 | -0.001 | 4.313038 |
| 0.000 | 10.841032 | 0.000 | 4.114475 | 0.000 | 5.006911 |
| 0.001 | 5.392167 | 0.001 | 2.791372 | 0.001 | 2.342821 |
| 0.002 | 2.687417 | 0.002 | 2.976505 | 0.002 | 3.084251 |
| 0.003 | 2.890587 | 0.003 | 3.174427 | 0.003 | 2.773897 |
| 0.004 | 1.863577 | 0.004 | 3.115664 | 0.004 | 1.315075 |
| 0.005 | 2.724660 | 0.005 | 1.517513 | 0.005 | 1.687608 |
| 0.006 | 3.088561 | 0.006 | 1.745767 | 0.006 | 4.179913 |
| 0.007 | 1.373843 | 0.007 | 5.462432 | 0.007 | 4.332564 |
| 0.008 | 2.256879 | 0.008 | 1.985788 | 0.008 | 4.356117 |
| 0.009 | 2.244569 | 0.009 | 2.215699 | 0.009 | 3.196826 |
| 0.010 | 2.349337 | 0.010 | 5.547042 | 0.010 | 2.207476 |
| 0.011 | 0.921578 | 0.011 | 2.158620 | 0.011 | 1.595290 |
| 0.012 | 0.000000 | 0.012 | 0.420510 | 0.012 | 0.263149 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| HOemim+ |  | MOEmim+ |  | PrSO3Hmim+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.013800 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 1.296877 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.638610 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.613331 |
| -0.017 | 0.590273 | -0.017 | 0.000000 | -0.017 | 1.126047 |
| -0.016 | 1.404444 | -0.016 | 0.000000 | -0.016 | 1.355653 |
| -0.015 | 1.516829 | -0.015 | 0.563479 | -0.015 | 0.905022 |
| -0.014 | 3.622328 | -0.014 | 2.864019 | -0.014 | 3.640372 |
| -0.013 | 3.392692 | -0.013 | 3.267570 | -0.013 | 4.059680 |
| -0.012 | 6.589685 | -0.012 | 4.977478 | -0.012 | 6.049531 |
| -0.011 | 10.653117 | -0.011 | 9.423689 | -0.011 | 10.605553 |
| -0.010 | 10.414639 | -0.010 | 8.919453 | -0.010 | 13.631369 |
| -0.009 | 15.786182 | -0.009 | 14.077953 | -0.009 | 23.802593 |
| -0.008 | 16.856466 | -0.008 | 14.590575 | -0.008 | 19.627134 |
| -0.007 | 18.091575 | -0.007 | 16.248427 | -0.007 | 20.199546 |
| -0.006 | 15.827069 | -0.006 | 19.068732 | -0.006 | 18.053302 |
| -0.005 | 22.123584 | -0.005 | 30.260054 | -0.005 | 20.100593 |
| -0.004 | 9.361722 | -0.004 | 17.021706 | -0.004 | 10.446266 |
| -0.003 | 6.310312 | -0.003 | 12.359663 | -0.003 | 7.801233 |
| -0.002 | 5.586682 | -0.002 | 11.886601 | -0.002 | 4.597259 |
| -0.001 | 3.315931 | -0.001 | 7.253892 | -0.001 | 4.915973 |
| 0.000 | 4.086623 | 0.000 | 5.397234 | 0.000 | 4.887372 |
| 0.001 | 2.869927 | 0.001 | 3.230490 | 0.001 | 3.580539 |
| 0.002 | 1.709631 | 0.002 | 0.950964 | 0.002 | 3.000852 |
| 0.003 | 0.823618 | 0.003 | 1.297577 | 0.003 | 3.041848 |
| 0.004 | 0.565726 | 0.004 | 0.785900 | 0.004 | 3.709788 |
| 0.005 | 1.190234 | 0.005 | 0.882334 | 0.005 | 4.177846 |
| 0.006 | 0.407920 | 0.006 | 1.260985 | 0.006 | 4.894339 |
| 0.007 | 1.032665 | 0.007 | 1.962772 | 0.007 | 8.412814 |
| 0.008 | 1.976080 | 0.008 | 1.771827 | 0.008 | 12.572353 |
| 0.009 | 0.919868 | 0.009 | 0.618118 | 0.009 | 8.297806 |
| 0.010 | 0.984499 | 0.010 | 1.140821 | 0.010 | 1.554894 |
| 0.011 | 1.555052 | 0.011 | 2.476554 | 0.011 | 0.000000 |
| 0.012 | 2.027380 | 0.012 | 0.387435 | 0.012 | 0.000000 |
| 0.013 | 1.890562 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.209650 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| Epy+ |  | BPy+ |  | HPy+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 1.037027 | -0.013 | 1.072450 | -0.013 | 0.999866 |
| -0.012 | 5.333860 | -0.012 | 5.200798 | -0.012 | 5.211717 |
| -0.011 | 6.025745 | -0.011 | 6.071710 | -0.011 | 6.149162 |
| -0.010 | 18.142029 | -0.010 | 17.742943 | -0.010 | 17.702291 |
| -0.009 | 18.019071 | -0.009 | 16.558582 | -0.009 | 16.501388 |
| -0.008 | 15.742725 | -0.008 | 14.011507 | -0.008 | 13.732289 |
| -0.007 | 16.883184 | -0.007 | 15.111338 | -0.007 | 15.132878 |
| -0.006 | 13.419114 | -0.006 | 11.063268 | -0.006 | 10.888663 |
| -0.005 | 16.132779 | -0.005 | 15.753411 | -0.005 | 15.356471 |
| -0.004 | 9.559698 | -0.004 | 17.780913 | -0.004 | 15.095145 |
| -0.003 | 12.113384 | -0.003 | 20.291949 | -0.003 | 25.092661 |
| -0.002 | 11.806134 | -0.002 | 19.333087 | -0.002 | 28.202819 |
| -0.001 | 10.473271 | -0.001 | 15.802300 | -0.001 | 27.302748 |
| 0.000 | 0.711982 | 0.000 | 7.513068 | 0.000 | 12.230050 |
| 0.001 | 0.000000 | 0.001 | 6.608890 | 0.001 | 10.965836 |
| 0.002 | 0.000000 | 0.002 | 4.321945 | 0.002 | 11.049161 |
| 0.003 | 0.000000 | 0.003 | 0.579540 | 0.003 | 3.151016 |
| 0.004 | 0.000000 | 0.004 | 0.000000 | 0.004 | 0.077443 |
| 0.005 | 0.000000 | 0.005 | 0.000000 | 0.005 | 0.000000 |
| 0.006 | 0.000000 | 0.006 | 0.000000 | 0.006 | 0.000000 |
| 0.007 | 0.000000 | 0.007 | 0.000000 | 0.007 | 0.000000 |
| 0.008 | 0.000000 | 0.008 | 0.000000 | 0.008 | 0.000000 |
| 0.009 | 0.000000 | 0.009 | 0.000000 | 0.009 | 0.000000 |
| 0.010 | 0.000000 | 0.010 | 0.000000 | 0.010 | 0.000000 |
| 0.011 | 0.000000 | 0.011 | 0.000000 | 0.011 | 0.000000 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 0.000000 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| OPy+ |  | PrSO3HPy+ |  | tmgh+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 1.078729 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.877523 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.474107 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.854651 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 1.658303 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.239217 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.595727 | -0.014 | 0.482896 |
| -0.013 | 1.097874 | -0.013 | 4.318539 | -0.013 | 2.734869 |
| -0.012 | 5.098120 | -0.012 | 6.799837 | -0.012 | 2.768443 |
| -0.011 | 6.107877 | -0.011 | 11.940107 | -0.011 | 2.335843 |
| -0.010 | 17.546171 | -0.010 | 29.353933 | -0.010 | 6.797385 |
| -0.009 | 16.503978 | -0.009 | 24.721617 | -0.009 | 12.199448 |
| -0.008 | 13.963169 | -0.008 | 17.476450 | -0.008 | 27.099989 |
| -0.007 | 15.112649 | -0.007 | 10.988553 | -0.007 | 23.318463 |
| -0.006 | 11.082573 | -0.006 | 9.516215 | -0.006 | 19.165407 |
| -0.005 | 15.113787 | -0.005 | 12.228276 | -0.005 | 20.542520 |
| -0.004 | 14.901901 | -0.004 | 10.482773 | -0.004 | 26.334459 |
| -0.003 | 25.234703 | -0.003 | 9.558131 | -0.003 | 12.450712 |
| -0.002 | 36.612131 | -0.002 | 9.859888 | -0.002 | 3.550319 |
| -0.001 | 36.792933 | -0.001 | 8.062683 | -0.001 | 1.500410 |
| 0.000 | 21.620444 | 0.000 | 1.693968 | 0.000 | 0.503687 |
| 0.001 | 16.030780 | 0.001 | 2.315619 | 0.001 | 0.549580 |
| 0.002 | 14.496786 | 0.002 | 3.484613 | 0.002 | 0.861515 |
| 0.003 | 7.086526 | 0.003 | 3.418102 | 0.003 | 0.605358 |
| 0.004 | 0.212895 | 0.004 | 4.097240 | 0.004 | 0.622234 |
| 0.005 | 0.000000 | 0.005 | 3.183851 | 0.005 | 0.132002 |
| 0.006 | 0.000000 | 0.006 | 5.079235 | 0.006 | 0.087977 |
| 0.007 | 0.000000 | 0.007 | 8.665121 | 0.007 | 0.639467 |
| 0.008 | 0.000000 | 0.008 | 12.412337 | 0.008 | 1.018996 |
| 0.009 | 0.000000 | 0.009 | 7.601747 | 0.009 | 0.250612 |
| 0.010 | 0.000000 | 0.010 | 0.701607 | 0.010 | 0.167716 |
| 0.011 | 0.000000 | 0.011 | 0.000000 | 0.011 | 0.143437 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 0.000000 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| N1111+ |  | N1222+ |  | N122,1O2+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 0.000000 |
| -0.012 | 2.081839 | -0.012 | 0.000000 | -0.012 | 0.407696 |
| -0.011 | 21.446576 | -0.011 | 1.346193 | -0.011 | 4.434174 |
| -0.010 | 24.984565 | -0.010 | 8.475601 | -0.010 | 13.894500 |
| -0.009 | 18.095061 | -0.009 | 19.983414 | -0.009 | 16.469747 |
| -0.008 | 18.319297 | -0.008 | 17.530158 | -0.008 | 17.956369 |
| -0.007 | 16.690482 | -0.007 | 21.509395 | -0.007 | 21.941227 |
| -0.006 | 9.755656 | -0.006 | 30.439748 | -0.006 | 29.970364 |
| -0.005 | 1.022981 | -0.005 | 27.023330 | -0.005 | 25.285849 |
| -0.004 | 0.000000 | -0.004 | 13.052430 | -0.004 | 16.898028 |
| -0.003 | 0.000000 | -0.003 | 9.712983 | -0.003 | 13.846410 |
| -0.002 | 0.000000 | -0.002 | 12.342012 | -0.002 | 16.740864 |
| -0.001 | 0.000000 | -0.001 | 8.058878 | -0.001 | 8.224223 |
| 0.000 | 0.000000 | 0.000 | 2.691499 | 0.000 | 3.708620 |
| 0.001 | 0.000000 | 0.001 | 0.000000 | 0.001 | 1.773983 |
| 0.002 | 0.000000 | 0.002 | 0.000000 | 0.002 | 0.893436 |
| 0.003 | 0.000000 | 0.003 | 0.000000 | 0.003 | 1.391553 |
| 0.004 | 0.000000 | 0.004 | 0.000000 | 0.004 | 1.031602 |
| 0.005 | 0.000000 | 0.005 | 0.000000 | 0.005 | 0.876664 |
| 0.006 | 0.000000 | 0.006 | 0.000000 | 0.006 | 1.223630 |
| 0.007 | 0.000000 | 0.007 | 0.000000 | 0.007 | 2.021129 |
| 0.008 | 0.000000 | 0.008 | 0.000000 | 0.008 | 1.541094 |
| 0.009 | 0.000000 | 0.009 | 0.000000 | 0.009 | 0.466439 |
| 0.010 | 0.000000 | 0.010 | 0.000000 | 0.010 | 1.666289 |
| 0.011 | 0.000000 | 0.011 | 0.000000 | 0.011 | 1.913411 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 0.117699 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| P2444+ |  | P4444+ |  | P4446+ |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 0.000000 |
| -0.012 | 0.000000 | -0.012 | 0.000000 | -0.012 | 0.000000 |
| -0.011 | 0.000000 | -0.011 | 0.000000 | -0.011 | 0.000000 |
| -0.010 | 4.268220 | -0.010 | 4.381981 | -0.010 | 4.578604 |
| -0.009 | 16.960401 | -0.009 | 17.478488 | -0.009 | 17.390875 |
| -0.008 | 12.552690 | -0.008 | 11.015150 | -0.008 | 10.789504 |
| -0.007 | 15.353666 | -0.007 | 13.878805 | -0.007 | 13.479273 |
| -0.006 | 23.236342 | -0.006 | 21.880450 | -0.006 | 21.877075 |
| -0.005 | 27.410977 | -0.005 | 25.334589 | -0.005 | 25.119885 |
| -0.004 | 38.602717 | -0.004 | 41.469457 | -0.004 | 39.019226 |
| -0.003 | 41.274251 | -0.003 | 49.426575 | -0.003 | 53.197266 |
| -0.002 | 39.834866 | -0.002 | 48.333397 | -0.002 | 57.291281 |
| -0.001 | 27.495840 | -0.001 | 30.514681 | -0.001 | 42.316428 |
| 0.000 | 26.437576 | 0.000 | 33.585504 | 0.000 | 38.768730 |
| 0.001 | 21.137900 | 0.001 | 28.159963 | 0.001 | 32.225625 |
| 0.002 | 15.904308 | 0.002 | 21.052457 | 0.002 | 27.441608 |
| 0.003 | 2.075501 | 0.003 | 2.774295 | 0.003 | 5.516859 |
| 0.004 | 0.000000 | 0.004 | 0.000000 | 0.004 | 0.102083 |
| 0.005 | 0.000000 | 0.005 | 0.000000 | 0.005 | 0.000000 |
| 0.006 | 0.000000 | 0.006 | 0.000000 | 0.006 | 0.000000 |
| 0.007 | 0.000000 | 0.007 | 0.000000 | 0.007 | 0.000000 |
| 0.008 | 0.000000 | 0.008 | 0.000000 | 0.008 | 0.000000 |
| 0.009 | 0.000000 | 0.009 | 0.000000 | 0.009 | 0.000000 |
| 0.010 | 0.000000 | 0.010 | 0.000000 | 0.010 | 0.000000 |
| 0.011 | 0.000000 | 0.011 | 0.000000 | 0.011 | 0.000000 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 0.000000 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| Anions | | | | | |
| Cl- |  | Br- |  | I- |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 0.000000 |
| -0.012 | 0.000000 | -0.012 | 0.000000 | -0.012 | 0.000000 |
| -0.011 | 0.000000 | -0.011 | 0.000000 | -0.011 | 0.000000 |
| -0.010 | 0.000000 | -0.010 | 0.000000 | -0.010 | 0.000000 |
| -0.009 | 0.000000 | -0.009 | 0.000000 | -0.009 | 0.000000 |
| -0.008 | 0.000000 | -0.008 | 0.000000 | -0.008 | 0.000000 |
| -0.007 | 0.000000 | -0.007 | 0.000000 | -0.007 | 0.000000 |
| -0.006 | 0.000000 | -0.006 | 0.000000 | -0.006 | 0.000000 |
| -0.005 | 0.000000 | -0.005 | 0.000000 | -0.005 | 0.000000 |
| -0.004 | 0.000000 | -0.004 | 0.000000 | -0.004 | 0.000000 |
| -0.003 | 0.000000 | -0.003 | 0.000000 | -0.003 | 0.000000 |
| -0.002 | 0.000000 | -0.002 | 0.000000 | -0.002 | 0.000000 |
| -0.001 | 0.000000 | -0.001 | 0.000000 | -0.001 | 0.000000 |
| 0.000 | 0.000000 | 0.000 | 0.000000 | 0.000 | 0.000000 |
| 0.001 | 0.000000 | 0.001 | 0.000000 | 0.001 | 0.000000 |
| 0.002 | 0.000000 | 0.002 | 0.000000 | 0.002 | 0.000000 |
| 0.003 | 0.000000 | 0.003 | 0.000000 | 0.003 | 0.000000 |
| 0.004 | 0.000000 | 0.004 | 0.000000 | 0.004 | 0.000000 |
| 0.005 | 0.000000 | 0.005 | 0.000000 | 0.005 | 0.000000 |
| 0.006 | 0.000000 | 0.006 | 0.000000 | 0.006 | 0.000000 |
| 0.007 | 0.000000 | 0.007 | 0.000000 | 0.007 | 0.000000 |
| 0.008 | 0.000000 | 0.008 | 0.000000 | 0.008 | 0.000000 |
| 0.009 | 0.000000 | 0.009 | 0.000000 | 0.009 | 0.000000 |
| 0.010 | 0.000000 | 0.010 | 0.000000 | 0.010 | 0.000000 |
| 0.011 | 0.000000 | 0.011 | 0.000000 | 0.011 | 0.000000 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 0.000000 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 16.367544 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 51.269699 |
| 0.016 | 0.000000 | 0.016 | 0.061821 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 56.462944 | 0.017 | 0.000000 |
| 0.018 | 4.477306 | 0.018 | 2.104902 | 0.018 | 0.000000 |
| 0.019 | 48.332874 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| Ac- |  | Pro- |  | TA- |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 0.000000 |
| -0.012 | 0.000000 | -0.012 | 0.000000 | -0.012 | 0.000000 |
| -0.011 | 0.000000 | -0.011 | 0.000000 | -0.011 | 0.000000 |
| -0.010 | 0.000000 | -0.010 | 0.000000 | -0.010 | 0.000000 |
| -0.009 | 0.000000 | -0.009 | 0.000000 | -0.009 | 0.000000 |
| -0.008 | 0.000000 | -0.008 | 0.000000 | -0.008 | 0.000000 |
| -0.007 | 0.000000 | -0.007 | 0.000000 | -0.007 | 0.000000 |
| -0.006 | 0.000000 | -0.006 | 0.000000 | -0.006 | 0.000000 |
| -0.005 | 0.000000 | -0.005 | 0.000000 | -0.005 | 0.000000 |
| -0.004 | 0.523799 | -0.004 | 0.000000 | -0.004 | 0.000000 |
| -0.003 | 2.318881 | -0.003 | 0.996273 | -0.003 | 0.000000 |
| -0.002 | 2.635514 | -0.002 | 5.543950 | -0.002 | 0.038996 |
| -0.001 | 4.588102 | -0.001 | 5.844134 | -0.001 | 0.413369 |
| 0.000 | 4.166339 | 0.000 | 8.831953 | 0.000 | 0.621672 |
| 0.001 | 3.516875 | 0.001 | 6.913227 | 0.001 | 0.607421 |
| 0.002 | 3.005717 | 0.002 | 7.703579 | 0.002 | 0.854881 |
| 0.003 | 6.442115 | 0.003 | 8.767776 | 0.003 | 8.162221 |
| 0.004 | 4.383675 | 0.004 | 6.560985 | 0.004 | 18.091525 |
| 0.005 | 2.794348 | 0.005 | 3.557611 | 0.005 | 23.980337 |
| 0.006 | 2.268412 | 0.006 | 2.255892 | 0.006 | 6.637687 |
| 0.007 | 1.625813 | 0.007 | 1.474348 | 0.007 | 3.404735 |
| 0.008 | 0.909613 | 0.008 | 1.627907 | 0.008 | 2.575320 |
| 0.009 | 2.046554 | 0.009 | 1.585559 | 0.009 | 1.885876 |
| 0.010 | 1.127697 | 0.010 | 1.057147 | 0.010 | 2.789492 |
| 0.011 | 1.018160 | 0.011 | 0.672595 | 0.011 | 2.666826 |
| 0.012 | 1.045811 | 0.012 | 0.977303 | 0.012 | 1.831489 |
| 0.013 | 1.359566 | 0.013 | 1.670970 | 0.013 | 2.499196 |
| 0.014 | 0.636386 | 0.014 | 1.041154 | 0.014 | 5.031814 |
| 0.015 | 0.859657 | 0.015 | 2.022380 | 0.015 | 12.777368 |
| 0.016 | 2.938755 | 0.016 | 1.960593 | 0.016 | 8.481360 |
| 0.017 | 3.490157 | 0.017 | 3.113830 | 0.017 | 4.238040 |
| 0.018 | 10.678947 | 0.018 | 8.809696 | 0.018 | 2.533633 |
| 0.019 | 9.127257 | 0.019 | 10.350924 | 0.019 | 2.578810 |
| 0.020 | 6.993590 | 0.020 | 5.362109 | 0.020 | 0.221045 |
| 0.021 | 3.879437 | 0.021 | 3.849461 | 0.021 | 0.000000 |
| 0.022 | 1.790262 | 0.022 | 1.651511 | 0.022 | 0.000000 |
| 0.023 | 1.933601 | 0.023 | 2.277778 | 0.023 | 0.000000 |
| 0.024 | 1.566862 | 0.024 | 1.413697 | 0.024 | 0.000000 |
| 0.025 | 0.678880 | 0.025 | 1.119375 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| Tos- |  | OTf- |  | MeSO4- |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 0.000000 |
| -0.012 | 0.000000 | -0.012 | 0.000000 | -0.012 | 0.000000 |
| -0.011 | 0.000000 | -0.011 | 0.000000 | -0.011 | 0.000000 |
| -0.010 | 0.000000 | -0.010 | 0.000000 | -0.010 | 0.000000 |
| -0.009 | 0.000000 | -0.009 | 0.000000 | -0.009 | 0.000000 |
| -0.008 | 0.000000 | -0.008 | 0.000000 | -0.008 | 0.000000 |
| -0.007 | 0.212568 | -0.007 | 0.000000 | -0.007 | 0.000000 |
| -0.006 | 3.695820 | -0.006 | 0.000000 | -0.006 | 1.203455 |
| -0.005 | 10.113003 | -0.005 | 0.000000 | -0.005 | 1.524745 |
| -0.004 | 11.556645 | -0.004 | 0.000000 | -0.004 | 3.433382 |
| -0.003 | 11.621517 | -0.003 | 0.000000 | -0.003 | 4.841015 |
| -0.002 | 7.490559 | -0.002 | 0.000000 | -0.002 | 5.369836 |
| -0.001 | 8.227174 | -0.001 | 0.000000 | -0.001 | 6.752617 |
| 0.000 | 11.147020 | 0.000 | 0.000000 | 0.000 | 2.817418 |
| 0.001 | 9.853044 | 0.001 | 1.015620 | 0.001 | 3.597862 |
| 0.002 | 5.123225 | 0.002 | 8.484619 | 0.002 | 1.296076 |
| 0.003 | 7.455506 | 0.003 | 20.997794 | 0.003 | 1.623382 |
| 0.004 | 3.757274 | 0.004 | 15.558014 | 0.004 | 1.804898 |
| 0.005 | 8.999211 | 0.005 | 6.129707 | 0.005 | 1.086347 |
| 0.006 | 9.206374 | 0.006 | 5.952571 | 0.006 | 1.237745 |
| 0.007 | 7.576290 | 0.007 | 3.580424 | 0.007 | 1.716027 |
| 0.008 | 2.992802 | 0.008 | 0.960829 | 0.008 | 1.074644 |
| 0.009 | 2.013425 | 0.009 | 3.105757 | 0.009 | 2.321141 |
| 0.010 | 3.056862 | 0.010 | 7.477340 | 0.010 | 3.737115 |
| 0.011 | 2.069932 | 0.011 | 15.400389 | 0.011 | 7.708757 |
| 0.012 | 3.872563 | 0.012 | 14.698850 | 0.012 | 10.924414 |
| 0.013 | 13.666116 | 0.013 | 13.966571 | 0.013 | 17.449604 |
| 0.014 | 11.313397 | 0.014 | 9.082024 | 0.014 | 19.363183 |
| 0.015 | 11.803302 | 0.015 | 0.015366 | 0.015 | 14.029166 |
| 0.016 | 14.402947 | 0.016 | 0.000000 | 0.016 | 1.548497 |
| 0.017 | 4.721576 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| EtSO4- |  | CH3OEtSO4- |  | PFBS- |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 0.000000 |
| -0.012 | 0.000000 | -0.012 | 0.000000 | -0.012 | 0.000000 |
| -0.011 | 0.000000 | -0.011 | 0.000000 | -0.011 | 0.000000 |
| -0.010 | 0.000000 | -0.010 | 0.000000 | -0.010 | 0.000000 |
| -0.009 | 0.000000 | -0.009 | 0.000000 | -0.009 | 0.000000 |
| -0.008 | 0.000000 | -0.008 | 0.000000 | -0.008 | 0.000000 |
| -0.007 | 0.000000 | -0.007 | 0.000000 | -0.007 | 0.000000 |
| -0.006 | 0.000000 | -0.006 | 0.857779 | -0.006 | 0.000000 |
| -0.005 | 1.079604 | -0.005 | 3.248326 | -0.005 | 0.000000 |
| -0.004 | 3.995888 | -0.004 | 13.169156 | -0.004 | 0.000000 |
| -0.003 | 8.266058 | -0.003 | 14.154416 | -0.003 | 0.000000 |
| -0.002 | 10.254813 | -0.002 | 11.020752 | -0.002 | 0.000000 |
| -0.001 | 8.233630 | -0.001 | 11.844214 | -0.001 | 1.030850 |
| 0.000 | 5.967751 | 0.000 | 8.558012 | 0.000 | 14.975558 |
| 0.001 | 8.554510 | 0.001 | 5.296380 | 0.001 | 51.075908 |
| 0.002 | 5.684970 | 0.002 | 3.319200 | 0.002 | 30.746503 |
| 0.003 | 1.749708 | 0.003 | 2.603542 | 0.003 | 20.302973 |
| 0.004 | 0.992812 | 0.004 | 2.197282 | 0.004 | 9.377656 |
| 0.005 | 0.922393 | 0.005 | 1.865049 | 0.005 | 7.369518 |
| 0.006 | 1.324247 | 0.006 | 2.362440 | 0.006 | 5.665075 |
| 0.007 | 1.516140 | 0.007 | 1.533224 | 0.007 | 4.032188 |
| 0.008 | 0.681779 | 0.008 | 3.176606 | 0.008 | 1.636340 |
| 0.009 | 2.168323 | 0.009 | 5.476935 | 0.009 | 3.325038 |
| 0.010 | 4.017518 | 0.010 | 5.390779 | 0.010 | 6.954954 |
| 0.011 | 7.515126 | 0.011 | 8.950015 | 0.011 | 11.451563 |
| 0.012 | 9.732501 | 0.012 | 15.132907 | 0.012 | 13.814768 |
| 0.013 | 16.267095 | 0.013 | 18.436617 | 0.013 | 12.598852 |
| 0.014 | 20.156007 | 0.014 | 18.744566 | 0.014 | 8.449444 |
| 0.015 | 15.466096 | 0.015 | 11.075015 | 0.015 | 0.383363 |
| 0.016 | 1.894316 | 0.016 | 0.543597 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| HSO4- |  | H2PO4- |  | Me2PO4- |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.215455 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.923854 | -0.015 | 1.770990 | -0.015 | 0.000000 |
| -0.014 | 0.285660 | -0.014 | 1.133909 | -0.014 | 0.000000 |
| -0.013 | 0.845072 | -0.013 | 1.104354 | -0.013 | 0.000000 |
| -0.012 | 0.916909 | -0.012 | 0.779905 | -0.012 | 0.000000 |
| -0.011 | 0.552556 | -0.011 | 1.660284 | -0.011 | 0.000000 |
| -0.010 | 0.421970 | -0.010 | 1.916137 | -0.010 | 0.000000 |
| -0.009 | 0.366176 | -0.009 | 0.859439 | -0.009 | 0.000000 |
| -0.008 | 0.926636 | -0.008 | 0.302758 | -0.008 | 0.000000 |
| -0.007 | 0.707509 | -0.007 | 0.864696 | -0.007 | 0.000000 |
| -0.006 | 0.427908 | -0.006 | 1.649867 | -0.006 | 0.596274 |
| -0.005 | 0.453719 | -0.005 | 1.380858 | -0.005 | 3.589142 |
| -0.004 | 0.178055 | -0.004 | 0.748217 | -0.004 | 6.186659 |
| -0.003 | 0.493734 | -0.003 | 0.722289 | -0.003 | 9.446399 |
| -0.002 | 0.234163 | -0.002 | 0.844535 | -0.002 | 10.446574 |
| -0.001 | 0.329332 | -0.001 | 0.777745 | -0.001 | 14.187980 |
| 0.000 | 0.404074 | 0.000 | 0.788107 | 0.000 | 8.370937 |
| 0.001 | 0.489425 | 0.001 | 0.610783 | 0.001 | 3.610618 |
| 0.002 | 0.591254 | 0.002 | 0.630604 | 0.002 | 4.658919 |
| 0.003 | 0.604297 | 0.003 | 1.413830 | 0.003 | 3.536881 |
| 0.004 | 0.994646 | 0.004 | 0.891968 | 0.004 | 4.417888 |
| 0.005 | 1.063704 | 0.005 | 1.276181 | 0.005 | 2.700741 |
| 0.006 | 1.999915 | 0.006 | 1.560769 | 0.006 | 1.177507 |
| 0.007 | 1.385215 | 0.007 | 1.165915 | 0.007 | 1.232649 |
| 0.008 | 1.094987 | 0.008 | 3.521826 | 0.008 | 2.283691 |
| 0.009 | 1.989532 | 0.009 | 4.554781 | 0.009 | 0.885000 |
| 0.010 | 4.888779 | 0.010 | 3.348855 | 0.010 | 1.429158 |
| 0.011 | 11.486034 | 0.011 | 3.032653 | 0.011 | 3.134299 |
| 0.012 | 11.471922 | 0.012 | 4.152586 | 0.012 | 2.262568 |
| 0.013 | 15.734339 | 0.013 | 7.233193 | 0.013 | 3.854522 |
| 0.014 | 21.206442 | 0.014 | 8.525515 | 0.014 | 13.501412 |
| 0.015 | 12.757919 | 0.015 | 7.559266 | 0.015 | 7.020006 |
| 0.016 | 0.492607 | 0.016 | 9.870889 | 0.016 | 4.461807 |
| 0.017 | 0.000000 | 0.017 | 11.155135 | 0.017 | 10.023621 |
| 0.018 | 0.000000 | 0.018 | 11.241716 | 0.018 | 8.608420 |
| 0.019 | 0.000000 | 0.019 | 2.356383 | 0.019 | 6.643674 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 3.350285 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.046079 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| FAP- |  | PF6- |  | BF4- |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 0.000000 |
| -0.012 | 0.000000 | -0.012 | 0.000000 | -0.012 | 0.000000 |
| -0.011 | 0.000000 | -0.011 | 0.000000 | -0.011 | 0.000000 |
| -0.010 | 0.000000 | -0.010 | 0.000000 | -0.010 | 0.000000 |
| -0.009 | 0.000000 | -0.009 | 0.000000 | -0.009 | 0.000000 |
| -0.008 | 0.000000 | -0.008 | 0.000000 | -0.008 | 0.000000 |
| -0.007 | 0.000000 | -0.007 | 0.000000 | -0.007 | 0.000000 |
| -0.006 | 0.000000 | -0.006 | 0.000000 | -0.006 | 0.000000 |
| -0.005 | 0.000000 | -0.005 | 0.000000 | -0.005 | 0.000000 |
| -0.004 | 0.000000 | -0.004 | 0.000000 | -0.004 | 0.000000 |
| -0.003 | 0.000000 | -0.003 | 0.000000 | -0.003 | 0.000000 |
| -0.002 | 0.000000 | -0.002 | 0.000000 | -0.002 | 0.000000 |
| -0.001 | 0.000000 | -0.001 | 0.000000 | -0.001 | 0.000000 |
| 0.000 | 0.000000 | 0.000 | 0.000000 | 0.000 | 0.000000 |
| 0.001 | 8.176141 | 0.001 | 0.000000 | 0.001 | 0.000000 |
| 0.002 | 46.000084 | 0.002 | 0.000000 | 0.002 | 0.000000 |
| 0.003 | 79.288422 | 0.003 | 0.000000 | 0.003 | 0.000000 |
| 0.004 | 50.214829 | 0.004 | 0.000000 | 0.004 | 0.000000 |
| 0.005 | 29.760876 | 0.005 | 0.270120 | 0.005 | 0.000000 |
| 0.006 | 12.809741 | 0.006 | 9.439218 | 0.006 | 0.000000 |
| 0.007 | 12.406164 | 0.007 | 15.089486 | 0.007 | 0.000000 |
| 0.008 | 8.535078 | 0.008 | 16.571871 | 0.008 | 0.000000 |
| 0.009 | 7.006177 | 0.009 | 28.985025 | 0.009 | 5.718927 |
| 0.010 | 1.779781 | 0.010 | 40.668297 | 0.010 | 20.253289 |
| 0.011 | 0.000000 | 0.011 | 3.264490 | 0.011 | 37.998969 |
| 0.012 | 0.000000 | 0.012 | 0.000000 | 0.012 | 24.945584 |
| 0.013 | 0.000000 | 0.013 | 0.000000 | 0.013 | 2.190850 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| TCB- |  | SbF6- |  | ClO4- |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 0.000000 |
| -0.012 | 0.000000 | -0.012 | 0.000000 | -0.012 | 0.000000 |
| -0.011 | 0.000000 | -0.011 | 0.000000 | -0.011 | 0.000000 |
| -0.010 | 0.000000 | -0.010 | 0.000000 | -0.010 | 0.000000 |
| -0.009 | 0.000000 | -0.009 | 0.000000 | -0.009 | 0.000000 |
| -0.008 | 0.000000 | -0.008 | 0.000000 | -0.008 | 0.000000 |
| -0.007 | 0.000000 | -0.007 | 0.000000 | -0.007 | 0.000000 |
| -0.006 | 0.000000 | -0.006 | 0.000000 | -0.006 | 0.000000 |
| -0.005 | 0.000000 | -0.005 | 0.000000 | -0.005 | 0.000000 |
| -0.004 | 1.360077 | -0.004 | 0.000000 | -0.004 | 0.000000 |
| -0.003 | 1.544199 | -0.003 | 0.000000 | -0.003 | 0.000000 |
| -0.002 | 3.037036 | -0.002 | 0.000000 | -0.002 | 0.000000 |
| -0.001 | 7.542037 | -0.001 | 0.000000 | -0.001 | 0.000000 |
| 0.000 | 3.895285 | 0.000 | 0.000000 | 0.000 | 0.000000 |
| 0.001 | 9.499657 | 0.001 | 0.000000 | 0.001 | 0.000000 |
| 0.002 | 12.177794 | 0.002 | 0.000000 | 0.002 | 0.000000 |
| 0.003 | 9.165401 | 0.003 | 0.000000 | 0.003 | 0.000000 |
| 0.004 | 6.003343 | 0.004 | 0.000000 | 0.004 | 0.000000 |
| 0.005 | 8.721450 | 0.005 | 3.651791 | 0.005 | 0.000000 |
| 0.006 | 7.500888 | 0.006 | 6.655797 | 0.006 | 0.283482 |
| 0.007 | 10.679663 | 0.007 | 36.919473 | 0.007 | 4.345531 |
| 0.008 | 19.839104 | 0.008 | 71.404262 | 0.008 | 5.970550 |
| 0.009 | 20.945456 | 0.009 | 12.627623 | 0.009 | 13.504765 |
| 0.010 | 17.230474 | 0.010 | 0.000000 | 0.010 | 9.286766 |
| 0.011 | 14.331052 | 0.011 | 0.000000 | 0.011 | 24.045286 |
| 0.012 | 7.666233 | 0.012 | 0.000000 | 0.012 | 33.242955 |
| 0.013 | 0.291366 | 0.013 | 0.000000 | 0.013 | 3.249174 |
| 0.014 | 0.000000 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 0.000000 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 0.000000 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 0.000000 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| NO3- |  | AlCl4- |  | FeCl4- |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 0.000000 |
| -0.012 | 0.000000 | -0.012 | 0.000000 | -0.012 | 0.000000 |
| -0.011 | 0.000000 | -0.011 | 0.000000 | -0.011 | 0.000000 |
| -0.010 | 0.000000 | -0.010 | 0.000000 | -0.010 | 0.000000 |
| -0.009 | 0.000000 | -0.009 | 0.000000 | -0.009 | 0.000000 |
| -0.008 | 0.000000 | -0.008 | 0.000000 | -0.008 | 0.000000 |
| -0.007 | 0.000000 | -0.007 | 0.000000 | -0.007 | 0.000000 |
| -0.006 | 0.000000 | -0.006 | 0.000000 | -0.006 | 0.000000 |
| -0.005 | 0.000000 | -0.005 | 0.000000 | -0.005 | 0.000000 |
| -0.004 | 0.000000 | -0.004 | 0.000000 | -0.004 | 0.000000 |
| -0.003 | 0.000000 | -0.003 | 0.000000 | -0.003 | 0.000000 |
| -0.002 | 0.000000 | -0.002 | 0.000000 | -0.002 | 0.000000 |
| -0.001 | 0.000000 | -0.001 | 0.000000 | -0.001 | 0.000000 |
| 0.000 | 0.000000 | 0.000 | 0.000000 | 0.000 | 0.000000 |
| 0.001 | 0.000000 | 0.001 | 0.000000 | 0.001 | 0.000000 |
| 0.002 | 0.125541 | 0.002 | 0.217533 | 0.002 | 0.765515 |
| 0.003 | 1.264019 | 0.003 | 7.571648 | 0.003 | 8.920961 |
| 0.004 | 0.361600 | 0.004 | 13.622315 | 0.004 | 10.622073 |
| 0.005 | 1.188776 | 0.005 | 26.372331 | 0.005 | 20.986575 |
| 0.006 | 2.134638 | 0.006 | 15.561290 | 0.006 | 15.302743 |
| 0.007 | 0.264078 | 0.007 | 46.241854 | 0.007 | 43.777351 |
| 0.008 | 1.964060 | 0.008 | 41.597650 | 0.008 | 51.138846 |
| 0.009 | 1.142606 | 0.009 | 4.256000 | 0.009 | 2.007027 |
| 0.010 | 4.012176 | 0.010 | 0.000000 | 0.010 | 0.000000 |
| 0.011 | 7.296523 | 0.011 | 0.000000 | 0.011 | 0.000000 |
| 0.012 | 9.564506 | 0.012 | 0.000000 | 0.012 | 0.000000 |
| 0.013 | 13.226225 | 0.013 | 0.000000 | 0.013 | 0.000000 |
| 0.014 | 7.785912 | 0.014 | 0.000000 | 0.014 | 0.000000 |
| 0.015 | 8.233807 | 0.015 | 0.000000 | 0.015 | 0.000000 |
| 0.016 | 5.443906 | 0.016 | 0.000000 | 0.016 | 0.000000 |
| 0.017 | 6.143616 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 4.541203 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 1.831983 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| SCN- |  | TCM- |  | DCA- |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 | -0.025 | 0.000000 |
| -0.024 | 0.000000 | -0.024 | 0.000000 | -0.024 | 0.000000 |
| -0.023 | 0.000000 | -0.023 | 0.000000 | -0.023 | 0.000000 |
| -0.022 | 0.000000 | -0.022 | 0.000000 | -0.022 | 0.000000 |
| -0.021 | 0.000000 | -0.021 | 0.000000 | -0.021 | 0.000000 |
| -0.020 | 0.000000 | -0.020 | 0.000000 | -0.020 | 0.000000 |
| -0.019 | 0.000000 | -0.019 | 0.000000 | -0.019 | 0.000000 |
| -0.018 | 0.000000 | -0.018 | 0.000000 | -0.018 | 0.000000 |
| -0.017 | 0.000000 | -0.017 | 0.000000 | -0.017 | 0.000000 |
| -0.016 | 0.000000 | -0.016 | 0.000000 | -0.016 | 0.000000 |
| -0.015 | 0.000000 | -0.015 | 0.000000 | -0.015 | 0.000000 |
| -0.014 | 0.000000 | -0.014 | 0.000000 | -0.014 | 0.000000 |
| -0.013 | 0.000000 | -0.013 | 0.000000 | -0.013 | 0.000000 |
| -0.012 | 0.000000 | -0.012 | 0.000000 | -0.012 | 0.000000 |
| -0.011 | 0.000000 | -0.011 | 0.000000 | -0.011 | 0.000000 |
| -0.010 | 0.000000 | -0.010 | 0.000000 | -0.010 | 0.000000 |
| -0.009 | 0.000000 | -0.009 | 0.000000 | -0.009 | 0.000000 |
| -0.008 | 0.000000 | -0.008 | 0.000000 | -0.008 | 0.000000 |
| -0.007 | 0.000000 | -0.007 | 0.000000 | -0.007 | 0.000000 |
| -0.006 | 0.000000 | -0.006 | 0.000000 | -0.006 | 0.000000 |
| -0.005 | 0.000000 | -0.005 | 0.000000 | -0.005 | 0.000000 |
| -0.004 | 0.000000 | -0.004 | 0.000000 | -0.004 | 0.000000 |
| -0.003 | 0.000000 | -0.003 | 0.000000 | -0.003 | 0.000000 |
| -0.002 | 0.000000 | -0.002 | 0.000000 | -0.002 | 0.000000 |
| -0.001 | 0.000000 | -0.001 | 0.000000 | -0.001 | 0.000000 |
| 0.000 | 0.000000 | 0.000 | 2.606592 | 0.000 | 0.000000 |
| 0.001 | 0.491567 | 0.001 | 11.883019 | 0.001 | 3.420654 |
| 0.002 | 0.775434 | 0.002 | 10.968972 | 0.002 | 2.593629 |
| 0.003 | 2.628148 | 0.003 | 12.518187 | 0.003 | 2.675594 |
| 0.004 | 0.006272 | 0.004 | 5.274101 | 0.004 | 6.968230 |
| 0.005 | 0.675191 | 0.005 | 6.427087 | 0.005 | 9.853895 |
| 0.006 | 3.558748 | 0.006 | 4.563381 | 0.006 | 8.162026 |
| 0.007 | 2.105868 | 0.007 | 4.870890 | 0.007 | 4.664381 |
| 0.008 | 0.158842 | 0.008 | 4.614428 | 0.008 | 3.279244 |
| 0.009 | 7.632657 | 0.009 | 9.136882 | 0.009 | 6.737040 |
| 0.010 | 15.081234 | 0.010 | 10.459383 | 0.010 | 3.198591 |
| 0.011 | 6.421402 | 0.011 | 14.496957 | 0.011 | 6.032945 |
| 0.012 | 11.463261 | 0.012 | 15.806444 | 0.012 | 3.737590 |
| 0.013 | 12.772534 | 0.013 | 13.865767 | 0.013 | 8.328778 |
| 0.014 | 3.580075 | 0.014 | 4.174351 | 0.014 | 11.595715 |
| 0.015 | 8.235912 | 0.015 | 0.000000 | 0.015 | 14.999288 |
| 0.016 | 8.260073 | 0.016 | 0.000000 | 0.016 | 6.009178 |
| 0.017 | 2.858153 | 0.017 | 0.000000 | 0.017 | 0.000000 |
| 0.018 | 0.000000 | 0.018 | 0.000000 | 0.018 | 0.000000 |
| 0.019 | 0.000000 | 0.019 | 0.000000 | 0.019 | 0.000000 |
| 0.020 | 0.000000 | 0.020 | 0.000000 | 0.020 | 0.000000 |
| 0.021 | 0.000000 | 0.021 | 0.000000 | 0.021 | 0.000000 |
| 0.022 | 0.000000 | 0.022 | 0.000000 | 0.022 | 0.000000 |
| 0.023 | 0.000000 | 0.023 | 0.000000 | 0.023 | 0.000000 |
| 0.024 | 0.000000 | 0.024 | 0.000000 | 0.024 | 0.000000 |
| 0.025 | 0.000000 | 0.025 | 0.000000 | 0.025 | 0.000000 |
|  |  |  |  |  |  |
| NTf2- |  | PhO- |  |  |  |
| -0.025 | 0.000000 | -0.025 | 0.000000 |  |  |
| -0.024 | 0.000000 | -0.024 | 0.000000 |  |  |
| -0.023 | 0.000000 | -0.023 | 0.000000 |  |  |
| -0.022 | 0.000000 | -0.022 | 0.000000 |  |  |
| -0.021 | 0.000000 | -0.021 | 0.000000 |  |  |
| -0.020 | 0.000000 | -0.020 | 0.000000 |  |  |
| -0.019 | 0.000000 | -0.019 | 0.000000 |  |  |
| -0.018 | 0.000000 | -0.018 | 0.000000 |  |  |
| -0.017 | 0.000000 | -0.017 | 0.000000 |  |  |
| -0.016 | 0.000000 | -0.016 | 0.000000 |  |  |
| -0.015 | 0.000000 | -0.015 | 0.000000 |  |  |
| -0.014 | 0.000000 | -0.014 | 0.000000 |  |  |
| -0.013 | 0.000000 | -0.013 | 0.000000 |  |  |
| -0.012 | 0.000000 | -0.012 | 0.000000 |  |  |
| -0.011 | 0.000000 | -0.011 | 0.000000 |  |  |
| -0.010 | 0.000000 | -0.010 | 0.000000 |  |  |
| -0.009 | 0.000000 | -0.009 | 0.000000 |  |  |
| -0.008 | 0.000000 | -0.008 | 0.000000 |  |  |
| -0.007 | 0.000000 | -0.007 | 0.000000 |  |  |
| -0.006 | 0.000000 | -0.006 | 0.000000 |  |  |
| -0.005 | 0.000000 | -0.005 | 0.130726 |  |  |
| -0.004 | 0.000000 | -0.004 | 2.881530 |  |  |
| -0.003 | 0.000000 | -0.003 | 4.759346 |  |  |
| -0.002 | 0.000000 | -0.002 | 8.440519 |  |  |
| -0.001 | 0.000000 | -0.001 | 5.493829 |  |  |
| 0.000 | 2.185200 | 0.000 | 7.769036 |  |  |
| 0.001 | 23.015610 | 0.001 | 5.574102 |  |  |
| 0.002 | 49.529052 | 0.002 | 4.472431 |  |  |
| 0.003 | 20.815136 | 0.003 | 4.727067 |  |  |
| 0.004 | 10.215222 | 0.004 | 5.741757 |  |  |
| 0.005 | 7.673198 | 0.005 | 2.297466 |  |  |
| 0.006 | 3.546665 | 0.006 | 5.181167 |  |  |
| 0.007 | 7.727300 | 0.007 | 6.920424 |  |  |
| 0.008 | 20.760791 | 0.008 | 4.802775 |  |  |
| 0.009 | 25.224138 | 0.009 | 6.448091 |  |  |
| 0.010 | 23.649056 | 0.010 | 10.936110 |  |  |
| 0.011 | 3.027737 | 0.011 | 8.959041 |  |  |
| 0.012 | 0.000000 | 0.012 | 7.608999 |  |  |
| 0.013 | 0.000000 | 0.013 | 3.427611 |  |  |
| 0.014 | 0.000000 | 0.014 | 0.502241 |  |  |
| 0.015 | 0.000000 | 0.015 | 0.324277 |  |  |
| 0.016 | 0.000000 | 0.016 | 1.186938 |  |  |
| 0.017 | 0.000000 | 0.017 | 0.122730 |  |  |
| 0.018 | 0.000000 | 0.018 | 1.626808 |  |  |
| 0.019 | 0.000000 | 0.019 | 4.864687 |  |  |
| 0.020 | 0.000000 | 0.020 | 4.440675 |  |  |
| 0.021 | 0.000000 | 0.021 | 4.669118 |  |  |
| 0.022 | 0.000000 | 0.022 | 3.773019 |  |  |
| 0.023 | 0.000000 | 0.023 | 1.665032 |  |  |
| 0.024 | 0.000000 | 0.024 | 0.000000 |  |  |
| 0.025 | 0.000000 | 0.025 | 0.000000 |  |  |

Table S5. The structures and names of the anions

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Number | Name | | Abbreviation | Structural | |
| 1 | Chloride | | Cl- | Cl | |
| 2 | Brimide | | Br- | Br | |
| 3 | Iodine | | I- |  | |
| 4 | Acetate | | Ac- | Ac | |
| 5 | Propionate | | Pro- |  | |
| 6 | Trifluoroacetate | | TA- | TA | |
| 7 | Tosylate | | Tos- | Tos | |
| 8 | Trifluoromethanesulfonate | | OTf- | OTf | |
| 9 | Methyl sulfate | | MeSO4- |  | |
| 10 | Ethyl sulfate | | EtSO4- |  | |
| 11 | Methoxyethyl sulfate | | CH3OEtSO4- |  | |
| 12 | Perfluorobutanesulfonate | | PFBS- |  | |
| 13 | Hydrogen sulfate | | HSO4- | HSO4 | |
| 14 | Dihydrogen phosphate | | H2PO4- | H2PO4 | |
| 15 | Dimethylphosphate | | Me2PO4- |  | |
| 16 | Perfluorophosphate | | FAP- |  | |
| 17 | Hexafluorophosphate | | PF6- |  | |
| 18 | Tetrafluoroborate | | BF4- | BF4 | |
| 19 | Boron cyanide | TCB- | | |  |
| 20 | Hexafluoroantimonate | SbF6- | | |  |
| 21 | Perchlorate | ClO4- | | | ClO4 |
| 22 | Nitrate | NO3- | | |  |
| 23 |  | AlCl4- | | |  |
| 24 |  | FeCl4- | | |  |
| 25 | Thiocyanate | SCN- | | |  |
| 26 | Tricyanomethane | TCM- | | |  |
| 27 | Dicyanamide | DCA- | | |  |
| 28 | Bis((trifluoromethyl)sulfonyl)imide | NTf2 | | |  |
| 29 | Phenoxy group | PhO- | | |  |

Table S6. The structures and names of the caions

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| No. | | Name | | | Abbreviation | Structural | |
| 1 | 1,3-Dimethylimidazolium | | Mmim+ |  | | |
| 2 | 1-Ethyl-3-methylimidazolium | | Emim+ |  | | |
| 3 | 1-Propyl-3-methylimidazolium | | Pmim+ |  | | |
| 4 | 1-Butyl-3-methylimidazolium | | Bmim+ |  | | |
| 5 | 1-Pentyl-3-methylimidazolium | | Pnmim+ |  | | |
| 6 | 1-Hexyl-3-methylimidazolium | | Hmim+ |  | | |
| 7 | 1-Octyl-3-methylimidazolium | | Omim+ |  | | |
| 8 | 1-Decyl-3-methylimidazolium | | Dmim+ |  | | |
| 9 | 1-Dodecyl-3-methylimidazolium | | C12-mim+ |  | | |
| 10 | 1-Tetradecyl-3-methylimidazolium | | C14-mim+ |  | | |
| 11 | 1-Hexadecyl-3-methylimidazolium | | C16-mim+ |  | | |
| 12 | 1-Allyl-3-methyl imidazolium | | Amim+ |  | | |
| 13 | 1-Benzyl-3-methyl imidazolium | | Bnmim+ |  | | |
| 14 | 1-Hydroxyethyl-3-methyl imidazolium | | HOemim+ |  | | |
| 15 | 1-Cyanopropyl-3-methyl imidazolium | | CPmim+ |  | | |
| 16 | 1-Aminopropyl-3-methyl imidazolium | | C3NH2mim+ |  | | |
| 17 | 1-((ethoxycarbonyl)methyl)-3-methyl imidazolium | | EOOEmim+ |  | | |
| 18 | 1-Methoxyethyl-3-methyl imidazolium | | MOEmim+ |  | | |
| 19 | 1-Carboxyethyl-3-methyl imidazolium | | HO2CEtmim+ |  | | |
| 20 | 1- Carboxymethyl -3-methyl imidazolium | | HO2CMmim+ |  | | |
| 21 | 1-Propylsulfonate-3-methyl imidazolium | | PrSO3Hmim+ |  | | |
| 22 | N-ethyl pyridinium | | EPy+ |  | | |
| 23 | N-butyl pyridinium | | BPy+ |  | | |
| 24 | N-butyl-3-metyl pyridinium | | BmPy+ |  | | |
| 25 | N-hexyl pyridinium | | HPy+ |  | | |
| 26 | N-octyl pyridinium | | OPy+ |  | | |
| 27 | N-propylsulfonate pyridinium | | PrSO3HPy+ |  | | |
| 28 | Tetramethyl ammonium | | N1111+ |  | | |
| 29 | Triethylmethyl ammonium | | N1222+ |  | | |
| 30 | N, N-diethyl-N-(2-methoxyethyl) ammonium | | N122,1O2+ |  | | |
| 31 | Tributylmethyl ammonium | | N1444+ |  | | |
| 32 | Methyltributyl phosphonium | | P1444+ |  | | |
| 33 | Ethyltributyl phosphonium | | P2444+ |  | | |
| 34 | Tetrabutyl phosphonium | | P4444+ |  | | |
| 35 | Tributylhexyl phosphonium | | P4446+ |  | | |
| 36 | N-butyl-N-methyl pyrrolidinium | | P14+ | P14 | | |
| 37 | N-butyl-N-methyl piperidinium | | PP14+ |  | | |
| 38 | N-methyl, butyl-Morpholinium | | BmMor+ |  | | |
| 39 |  | | Tmgh+ |  | | |

Table S7. The calculated results of the distribution coefficients (*D*), selectivity (*S*), extractant cost (*SL*) and the solvent’s solubility (*SP*) for 418 ILs to extract indole at 298.15 K

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Cations | | Anions | | | | *D* | | | *S* | | | | | | *SL* | | | | | | | *SP* | | | | | | | |
| Emin+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 74011.26 | | | 41573.38 | | | | | | 1.79E-11 | | | | | | | 45886.31 | | | | | | | |
|  | | Ac- | | | | 34908.94 | | | 57914.84 | | | | | | 2.38E-11 | | | | | | | 21643.22 | | | | | | | |
|  | | TA- | | | | 222.71 | | | 1223.35 | | | | | | 3.74E-08 | | | | | | | 138.08 | | | | | | | |
|  | | Tos- | | | | 346.41 | | | 935.85 | | | | | | 1.12E-07 | | | | | | | 214.77 | | | | | | | |
|  | | OTf- | | | | 14.54 | | | 94.47 | | | | | | 9.47E-06 | | | | | | | 9.01 | | | | | | | |
|  | | MeSO4- | | | | 129.91 | | | 557.53 | | | | | | 1.77E-07 | | | | | | | 80.55 | | | | | | | |
|  | | CH3OEtSO4- | | | | 115.49 | | | 361.05 | | | | | | 7.46E-07 | | | | | | | 71.60 | | | | | | | |
|  | | PFBS- | | | | 21.84 | | | 44.47 | | | | | | 1.43E-04 | | | | | | | 13.54 | | | | | | | |
|  | | HSO4- | | | | 81.30 | | | 513.51 | | | | | | 7.23E-09 | | | | | | | 50.40 | | | | | | | |
|  | | H2PO4- | | | | 1002.82 | | | 3384.84 | | | | | | 2.05E-12 | | | | | | | 621.74 | | | | | | | |
|  | | Me2PO4- | | | | 3161.28 | | | 7500.26 | | | | | | 1.20E-09 | | | | | | | 1959.96 | | | | | | | |
|  | | BF4- | | | | 9.78 | | | 86.59 | | | | | | 5.95E-06 | | | | | | | 6.06 | | | | | | | |
|  | | ClO4- | | | | 9.61 | | | 87.56 | | | | | | 6.42E-06 | | | | | | | 5.96 | | | | | | | |
|  | | NO3- | | | | 668.77 | | | 2273.92 | | | | | | 8.57E-09 | | | | | | | 414.63 | | | | | | | |
|  | | SCN- | | | | 126.84 | | | 700.08 | | | | | | 1.05E-07 | | | | | | | 78.64 | | | | | | | |
|  | | TCM- | | | | 11.53 | | | 68.94 | | | | | | 1.99E-05 | | | | | | | 7.15 | | | | | | | |
|  | | DCA- | | | | 77.01 | | | 507.35 | | | | | | 2.05E-07 | | | | | | | 47.75 | | | | | | | |
|  | | NTf2- | | | | 3.02 | | | 4.22 | | | | | | 2.49E-02 | | | | | | | 1.87 | | | | | | | |
|  | | PhO- | | | | 3591.40 | | | 9817.39 | | | | | | 8.28E-10 | | | | | | | 2226.63 | | | | | | | |
| Bmim+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 12093.27 | | | 29456.25 | | | | | | 1.56E-14 | | | | | | | 7497.72 | | | | | | | |
|  | | Ac- | | | | 7429.91 | | | 21266.80 | | | | | | 5.25E-14 | | | | | | | 4606.47 | | | | | | | |
|  | | TA- | | | | 109.02 | | | 460.14 | | | | | | 1.03E-09 | | | | | | | 67.59 | | | | | | | |
|  | | Tos- | | | | 209.95 | | | 541.23 | | | | | | 2.64E-09 | | | | | | | 130.16 | | | | | | | |
|  | | OTf- | | | | 12.02 | | | 50.98 | | | | | | 1.96E-06 | | | | | | | 7.46 | | | | | | | |
|  | | MeSO4- | | | | 69.22 | | | 332.01 | | | | | | 8.47E-09 | | | | | | | 42.92 | | | | | | | |
|  | | CH3OEtSO4- | | | | 74.65 | | | 226.20 | | | | | | 4.37E-08 | | | | | | | 46.28 | | | | | | | |
|  | | PFBS- | | | | 15.46 | | | 26.64 | | | | | | 2.26E-05 | | | | | | | 9.58 | | | | | | | |
|  | | HSO4- | | | | 34.93 | | | 295.49 | | | | | | 4.46E-10 | | | | | | | 21.66 | | | | | | | |
|  | | H2PO4- | | | | 278.33 | | | 1728.75 | | | | | | 2.10E-14 | | | | | | | 172.56 | | | | | | | |
|  | | Me2PO4- | | | | 1302.38 | | | 3705.38 | | | | | | 7.31E-12 | | | | | | | 807.47 | | | | | | | |
|  | | BF4- | | | | 6.14 | | | 50.01 | | | | | | 2.22E-06 | | | | | | | 3.81 | | | | | | | |
|  | | ClO4- | | | | 6.41 | | | 49.34 | | | | | | 2.32E-06 | | | | | | | 3.98 | | | | | | | |
|  | | NO3- | | | | 168.94 | | | 989.07 | | | | | | 1.55E-10 | | | | | | | 104.74 | | | | | | | |
|  | | SCN- | | | | 48.09 | | | 312.20 | | | | | | 5.37E-09 | | | | | | | 29.82 | | | | | | | |
|  | | TCM- | | | | 9.64 | | | 38.04 | | | | | | 5.26E-06 | | | | | | | 5.97 | | | | | | | |
|  | | DCA- | | | | 43.85 | | | 244.33 | | | | | | 1.15E-08 | | | | | | | 27.18 | | | | | | | |
|  | | NTf2- | | | | 2.93 | | | 3.15 | | | | | | 2.81E-02 | | | | | | | 1.82 | | | | | | | |
|  | | PhO- | | | | 666.59 | | | 1785.95 | | | | | | 9.53E-12 | | | | | | | 413.28 | | | | | | | |
| Amim+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 60349.57 | | | 41423.34 | | | | | | 1.27E-11 | | | | | | | 37416.18 | | | | | | | |
|  | | Ac- | | | | 30740.03 | | | 55512.48 | | | | | | 1.93E-11 | | | | | | | 19058.54 | | | | | | | |
|  | | TA- | | | | 212.25 | | | 1123.84 | | | | | | 3.35E-08 | | | | | | | 131.59 | | | | | | | |
|  | | Tos- | | | | 327.35 | | | 875.10 | | | | | | 9.46E-08 | | | | | | | 202.96 | | | | | | | |
|  | | OTf- | | | | 14.47 | | | 85.82 | | | | | | 9.43E-06 | | | | | | | 8.97 | | | | | | | |
|  | | MeSO4- | | | | 114.59 | | | 517.50 | | | | | | 1.46E-07 | | | | | | | 71.04 | | | | | | | |
|  | | CH3OEtSO4- | | | | 106.62 | | | 335.86 | | | | | | 6.29E-07 | | | | | | | 66.10 | | | | | | | |
|  | | PFBS- | | | | 22.31 | | | 41.90 | | | | | | 1.43E-04 | | | | | | | 13.83 | | | | | | | |
|  | | HSO4- | | | | 67.48 | | | 480.17 | | | | | | 6.03E-09 | | | | | | | 41.84 | | | | | | | |
|  | | H2PO4- | | | | 849.44 | | | 3259.96 | | | | | | 1.58E-12 | | | | | | | 526.65 | | | | | | | |
|  | | Me2PO4- | | | | 2911.95 | | | 7017.86 | | | | | | 9.37E-10 | | | | | | | 1805.38 | | | | | | | |
|  | | BF4- | | | | 8.10 | | | 79.45 | | | | | | 5.32E-06 | | | | | | | 5.02 | | | | | | | |
|  | | ClO4- | | | | 8.05 | | | 80.17 | | | | | | 5.75E-06 | | | | | | | 4.99 | | | | | | | |
|  | | NO3- | | | | 530.97 | | | 2129.32 | | | | | | 6.35E-09 | | | | | | | 329.20 | | | | | | | |
|  | | SCN- | | | | 104.54 | | | 649.53 | | | | | | 8.45E-08 | | | | | | | 64.81 | | | | | | | |
|  | | TCM- | | | | 11.42 | | | 62.83 | | | | | | 1.96E-05 | | | | | | | 7.08 | | | | | | | |
|  | | DCA- | | | | 69.64 | | | 467.81 | | | | | | 1.81E-07 | | | | | | | 43.18 | | | | | | | |
|  | | NTf2- | | | | 3.10 | | | 4.00 | | | | | | 2.68E-02 | | | | | | | 1.92 | | | | | | | |
|  | | PhO- | | | | 3315.48 | | | 9249.28 | | | | | | 6.53E-10 | | | | | | | 2055.57 | | | | | | | |
| Bnmim+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 27983.80 | | | 35888.15 | | | | | | 5.31E-11 | | | | | | | 17349.70 | | | | | | | |
|  | | Ac- | | | | 27098.94 | | | 51597.32 | | | | | | 1.12E-10 | | | | | | | 16801.10 | | | | | | | |
|  | | TA- | | | | 295.89 | | | 1002.11 | | | | | | 1.52E-07 | | | | | | | 183.45 | | | | | | | |
|  | | Tos- | | | | 369.75 | | | 769.55 | | | | | | 3.51E-07 | | | | | | | 229.24 | | | | | | | |
|  | | OTf- | | | | 20.54 | | | 71.17 | | | | | | 3.22E-05 | | | | | | | 12.74 | | | | | | | |
|  | | MeSO4- | | | | 121.97 | | | 424.61 | | | | | | 5.35E-07 | | | | | | | 75.62 | | | | | | | |
|  | | CH3OEtSO4- | | | | 119.05 | | | 285.56 | | | | | | 2.10E-06 | | | | | | | 73.81 | | | | | | | |
|  | | PFBS- | | | | 27.69 | | | 38.66 | | | | | | 3.71E-04 | | | | | | | 17.17 | | | | | | | |
|  | | HSO4- | | | | 67.88 | | | 385.57 | | | | | | 2.46E-08 | | | | | | | 42.09 | | | | | | | |
|  | | H2PO4- | | | | 735.40 | | | 2882.26 | | | | | | 7.39E-12 | | | | | | | 455.94 | | | | | | | |
|  | | Me2PO4- | | | | 3037.81 | | | 6322.04 | | | | | | 4.26E-09 | | | | | | | 1883.41 | | | | | | | |
|  | | BF4- | | | | 9.62 | | | 59.28 | | | | | | 1.85E-05 | | | | | | | 5.96 | | | | | | | |
|  | | ClO4- | | | | 10.03 | | | 60.14 | | | | | | 2.04E-05 | | | | | | | 6.22 | | | | | | | |
|  | | NO3- | | | | 481.17 | | | 1839.70 | | | | | | 2.58E-08 | | | | | | | 298.32 | | | | | | | |
|  | | SCN- | | | | 114.69 | | | 538.36 | | | | | | 3.33E-07 | | | | | | | 71.11 | | | | | | | |
|  | | TCM- | | | | 16.16 | | | 52.36 | | | | | | 6.44E-05 | | | | | | | 10.02 | | | | | | | |
|  | | DCA- | | | | 89.72 | | | 385.63 | | | | | | 7.57E-07 | | | | | | | 55.63 | | | | | | | |
|  | | NTf2- | | | | 3.63 | | | 3.58 | | | | | | 5.00E-02 | | | | | | | 2.25 | | | | | | | |
|  | | PhO- | | | | 4797.33 | | | 10473.05 | | | | | | 3.39E-09 | | | | | | | 2974.30 | | | | | | | |
| C3NH2mim+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 48706.09 | | | 35436.17 | | | | | | 2.96E-12 | | | | | | | 30197.33 | | | | | | | |
|  | | Ac- | | | | 29257.66 | | | 48926.39 | | | | | | 4.97E-12 | | | | | | | 18139.48 | | | | | | | |
|  | | TA- | | | | 314.57 | | | 1495.27 | | | | | | 6.88E-09 | | | | | | | 195.03 | | | | | | | |
|  | | Tos- | | | | 476.63 | | | 1205.52 | | | | | | 1.96E-08 | | | | | | | 295.50 | | | | | | | |
|  | | OTf- | | | | 36.50 | | | 202.92 | | | | | | 9.78E-07 | | | | | | | 22.63 | | | | | | | |
|  | | MeSO4- | | | | 218.57 | | | 832.41 | | | | | | 2.60E-08 | | | | | | | 135.51 | | | | | | | |
|  | | CH3OEtSO4- | | | | 201.19 | | | 579.10 | | | | | | 1.06E-07 | | | | | | | 124.74 | | | | | | | |
|  | | PFBS- | | | | 50.39 | | | 102.64 | | | | | | 1.42E-05 | | | | | | | 31.24 | | | | | | | |
|  | | HSO4- | | | | 127.13 | | | 685.41 | | | | | | 9.98E-10 | | | | | | | 78.82 | | | | | | | |
|  | | H2PO4- | | | | 1088.52 | | | 3491.79 | | | | | | 4.06E-13 | | | | | | | 674.87 | | | | | | | |
|  | | Me2PO4- | | | | 3241.39 | | | 7290.69 | | | | | | 2.44E-10 | | | | | | | 2009.63 | | | | | | | |
|  | | BF4- | | | | 31.40 | | | 216.03 | | | | | | 5.28E-07 | | | | | | | 19.47 | | | | | | | |
|  | | ClO4- | | | | 30.15 | | | 213.62 | | | | | | 5.75E-07 | | | | | | | 18.69 | | | | | | | |
|  | | NO3- | | | | 794.18 | | | 2577.06 | | | | | | 1.52E-09 | | | | | | | 492.39 | | | | | | | |
|  | | SCN- | | | | 202.86 | | | 967.55 | | | | | | 1.63E-08 | | | | | | | 125.77 | | | | | | | |
|  | | TCM- | | | | 30.97 | | | 160.31 | | | | | | 1.86E-06 | | | | | | | 19.20 | | | | | | | |
|  | | DCA- | | | | 134.86 | | | 742.02 | | | | | | 3.14E-08 | | | | | | | 83.61 | | | | | | | |
|  | | NTf2- | | | | 13.59 | | | 20.61 | | | | | | 9.29E-04 | | | | | | | 8.42 | | | | | | | |
|  | | PhO- | | | | 3926.11 | | | 10081.88 | | | | | | 1.87E-10 | | | | | | | 2434.15 | | | | | | | |
| Cpmim+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 29057.04 | | | 17169.19 | | | | | | 1.15E-14 | | | | | | | 18015.10 | | | | | | | |
|  | | Ac- | | | | 8840.46 | | | 21335.48 | | | | | | 4.03E-14 | | | | | | | 5481.00 | | | | | | | |
|  | | TA- | | | | 65.01 | | | 777.34 | | | | | | 2.62E-10 | | | | | | | 40.31 | | | | | | | |
|  | | Tos- | | | | 128.09 | | | 608.60 | | | | | | 6.16E-10 | | | | | | | 79.41 | | | | | | | |
|  | | OTf- | | | | 5.72 | | | 84.83 | | | | | | 1.22E-07 | | | | | | | 3.55 | | | | | | | |
|  | | MeSO4- | | | | 47.16 | | | 409.38 | | | | | | 7.97E-10 | | | | | | | 29.24 | | | | | | | |
|  | | CH3OEtSO4- | | | | 45.77 | | | 271.12 | | | | | | 4.72E-09 | | | | | | | 28.38 | | | | | | | |
|  | | PFBS- | | | | 12.51 | | | 40.19 | | | | | | 4.42E-06 | | | | | | | 7.76 | | | | | | | |
|  | | HSO4- | | | | 31.98 | | | 399.71 | | | | | | 3.25E-11 | | | | | | | 19.82 | | | | | | | |
|  | | H2PO4- | | | | 406.79 | | | 2052.81 | | | | | | 6.35E-15 | | | | | | | 252.20 | | | | | | | |
|  | | Me2PO4- | | | | 946.42 | | | 3657.23 | | | | | | 2.77E-12 | | | | | | | 586.77 | | | | | | | |
|  | | BF4- | | | | 3.83 | | | 90.03 | | | | | | 4.24E-08 | | | | | | | 2.38 | | | | | | | |
|  | | ClO4- | | | | 3.64 | | | 90.41 | | | | | | 4.89E-08 | | | | | | | 2.26 | | | | | | | |
|  | | NO3- | | | | 221.15 | | | 1387.38 | | | | | | 2.63E-11 | | | | | | | 137.11 | | | | | | | |
|  | | SCN- | | | | 41.93 | | | 512.93 | | | | | | 5.17E-10 | | | | | | | 26.00 | | | | | | | |
|  | | TCM- | | | | 4.85 | | | 64.96 | | | | | | 2.83E-07 | | | | | | | 3.01 | | | | | | | |
|  | | DCA- | | | | 24.83 | | | 381.23 | | | | | | 1.32E-09 | | | | | | | 15.39 | | | | | | | |
|  | | NTf2- | | | | 2.82 | | | 6.53 | | | | | | 1.05E-03 | | | | | | | 1.75 | | | | | | | |
|  | | PhO- | | | | 888.75 | | | 4535.29 | | | | | | 5.39E-12 | | | | | | | 551.02 | | | | | | | |
| EOOEmim+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 10648.81 | | | 20470.42 | | | | | | 5.67E-14 | | | | | | | 6602.16 | | | | | | | |
|  | | Ac- | | | | 7095.07 | | | 19447.64 | | | | | | 1.60E-13 | | | | | | | 4398.88 | | | | | | | |
|  | | | | | TA- | | 102.30 | | | | 521.60 | | | | | | 4.97E-09 | | | | | | | 63.43 | | | | | | | |
|  | | | | | Tos- | | 177.82 | | | | 518.75 | | | | | | 9.32E-09 | | | | | | | 110.25 | | | | | | | |
|  | | | | | OTf- | | 10.85 | | | | 58.16 | | | | | | 3.04E-06 | | | | | | | 6.73 | | | | | | | |
|  | | | | | MeSO4- | | 60.76 | | | | 326.76 | | | | | | 1.79E-08 | | | | | | | 37.67 | | | | | | | |
|  | | | | | CH3OEtSO4- | | 64.71 | | | | 224.72 | | | | | | 9.07E-08 | | | | | | | 40.12 | | | | | | | |
|  | | | | | PFBS- | | 16.00 | | | | 30.53 | | | | | | 5.02E-05 | | | | | | | 9.92 | | | | | | | |
|  | | | | | HSO4- | | 32.92 | | | | 299.30 | | | | | | 8.87E-10 | | | | | | | 20.41 | | | | | | | |
|  | | | | | H2PO4- | | 277.64 | | | | 1650.39 | | | | | | 9.86E-14 | | | | | | | 172.13 | | | | | | | |
|  | | | | | Me2PO4- | | 1113.51 | | | | 3348.95 | | | | | | 3.28E-11 | | | | | | | 690.36 | | | | | | | |
|  | | | | | BF4- | | 5.63 | | | | 56.14 | | | | | | 1.76E-06 | | | | | | | 3.49 | | | | | | | |
|  | | | | | ClO4- | | 5.80 | | | | 55.80 | | | | | | 1.98E-06 | | | | | | | 3.59 | | | | | | | |
|  | | | | | NO3- | | 176.56 | | | | 1074.33 | | | | | | 5.81E-10 | | | | | | | 109.47 | | | | | | | |
|  | | | | | SCN- | | 47.60 | | | | 353.83 | | | | | | 1.49E-08 | | | | | | | 29.51 | | | | | | | |
|  | | | | | TCM- | | 8.90 | | | | 44.24 | | | | | | 7.13E-06 | | | | | | | 5.52 | | | | | | | |
|  | | | | | DCA- | | 38.31 | | | | 257.94 | | | | | | 3.21E-08 | | | | | | | 23.75 | | | | | | | |
|  | | | | | NTf2- | | 3.15 | | | | 3.95 | | | | | | 1.71E-02 | | | | | | | 1.95 | | | | | | | |
|  | | | | | PhO- | | 802.53 | | | | 2431.49 | | | | | | 5.66E-11 | | | | | | | 497.56 | | | | | | | |
| HO2CEtmim+ | | | | |  | |  | | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | | | | Cl- | | 7796.40 | | | | 13323.24 | | | | | | 5.16E-18 | | | | | | | 4833.70 | | | | | | | |
|  | | | | | Ac- | | 1795.43 | | | | 8018.53 | | | | | | 8.22E-17 | | | | | | | 1113.15 | | | | | | | |
|  | | | | | TA- | | 24.19 | | | | 336.07 | | | | | | 1.58E-12 | | | | | | | 15.00 | | | | | | | |
|  | | | | | Tos- | | 68.96 | | | | 401.09 | | | | | | 2.17E-12 | | | | | | | 42.75 | | | | | | | |
|  | | | | | OTf- | | 3.49 | | | | 52.87 | | | | | | 4.67E-09 | | | | | | | 2.16 | | | | | | | |
|  | | | | | MeSO4- | | 21.08 | | | | 299.51 | | | | | | 4.79E-12 | | | | | | | 13.07 | | | | | | | |
|  | | | | | CH3OEtSO4- | | 25.78 | | | | 198.93 | | | | | | 3.83E-11 | | | | | | | 15.98 | | | | | | | |
|  | | | | | PFBS- | | 7.93 | | | | 25.21 | | | | | | 1.68E-07 | | | | | | | 4.91 | | | | | | | |
|  | | | | | HSO4- | | 10.80 | | | | 297.91 | | | | | | 2.19E-13 | | | | | | | 6.70 | | | | | | | |
|  | | | | | H2PO4- | | 110.28 | | | | 1278.70 | | | | | | 1.25E-17 | | | | | | | 68.38 | | | | | | | |
|  | | | | | Me2PO4- | | 358.98 | | | | 2034.32 | | | | | | 5.23E-15 | | | | | | | 222.57 | | | | | | | |
|  | | | | | BF4- | | 1.50 | | | | 68.52 | | | | | | 3.28E-09 | | | | | | | 0.93 | | | | | | | |
|  | | | | | ClO4- | | 1.51 | | | | 66.57 | | | | | | 3.55E-09 | | | | | | | 0.94 | | | | | | | |
|  | | | | | NO3- | | 49.92 | | | | 750.74 | | | | | | 8.68E-14 | | | | | | | 30.95 | | | | | | | |
|  | | | | | SCN- | | 12.09 | | | | 293.76 | | | | | | 3.23E-12 | | | | | | | 7.50 | | | | | | | |
|  | | | | | TCM- | | 2.98 | | | | 40.91 | | | | | | 1.54E-08 | | | | | | | 1.84 | | | | | | | |
|  | | | | | DCA- | | 10.47 | | | | 228.36 | | | | | | 9.02E-12 | | | | | | | 6.49 | | | | | | | |
|  | | | | | NTf2- | | 2.07 | | | | 4.21 | | | | | | 8.70E-04 | | | | | | | 1.29 | | | | | | | |
|  | | | | | PhO- | | 173.96 | | | | 1151.99 | | | | | | 4.43E-14 | | | | | | | 107.85 | | | | | | | |
| HOemim+ | | | | |  | |  | | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | | | | Cl- | | 25132.53 | | | | 18835.07 | | | | | | 2.05E-16 | | | | | | | 15581.94 | | | | | | | |
|  | | | | | Ac- | | 4908.69 | | | | 14294.70 | | | | | | 1.23E-15 | | | | | | | 3043.34 | | | | | | | |
|  | | | | | TA- | | 40.51 | | | | 544.89 | | | | | | 1.34E-11 | | | | | | | 25.11 | | | | | | | |
|  | | | | | Tos- | | 106.96 | | | | 558.89 | | | | | | 3.22E-11 | | | | | | | 66.32 | | | | | | | |
|  | | | | | OTf- | | 4.61 | | | | 75.79 | | | | | | 2.43E-08 | | | | | | | 2.86 | | | | | | | |
|  | | | | MeSO4- | | | 37.98 | | | 404.02 | | | | | | 7.23E-11 | | | | | | | 23.55 | | | | | | | |
|  | | | | CH3OEtSO4- | | | 39.71 | | | 264.83 | | | | | | 4.99E-10 | | | | | | | 24.62 | | | | | | | |
|  | | | | PFBS- | | | 10.08 | | | 34.18 | | | | | | 7.67E-07 | | | | | | | 6.25 | | | | | | | |
|  | | | | HSO4- | | | 23.44 | | | 392.83 | | | | | | 3.08E-12 | | | | | | | 14.53 | | | | | | | |
|  | | | | H2PO4- | | | 266.75 | | | 1768.80 | | | | | | 2.14E-16 | | | | | | | 165.38 | | | | | | | |
|  | | | | Me2PO4- | | | 688.65 | | | 3127.91 | | | | | | 9.09E-14 | | | | | | | 426.96 | | | | | | | |
|  | | | | BF4- | | | 2.97 | | | 92.33 | | | | | | 1.45E-08 | | | | | | | 1.84 | | | | | | | |
|  | | | | ClO4- | | | 2.82 | | | 91.03 | | | | | | 1.57E-08 | | | | | | | 1.75 | | | | | | | |
|  | | | | NO3- | | | 136.52 | | | 1112.97 | | | | | | 1.34E-12 | | | | | | | 84.64 | | | | | | | |
|  | | | | SCN- | | | 27.50 | | | 428.81 | | | | | | 4.05E-11 | | | | | | | 17.05 | | | | | | | |
|  | | | | TCM- | | | 3.92 | | | 58.12 | | | | | | 6.76E-08 | | | | | | | 2.43 | | | | | | | |
|  | | | | DCA- | | | 17.91 | | | 332.01 | | | | | | 1.02E-10 | | | | | | | 11.11 | | | | | | | |
|  | | | | NTf2- | | | 2.49 | | | 5.48 | | | | | | 8.33E-04 | | | | | | | 1.55 | | | | | | | |
|  | | | | PhO- | | | 371.31 | | | 2091.57 | | | | | | 3.12E-13 | | | | | | | 230.21 | | | | | | | |
| MOEmim+ | | | |  | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | | | Cl- | | | 32929.14 | | | 33763.04 | | | | | | 1.16E-12 | | | | | | | 20415.77 | | | | | | | |
|  | | | | Ac- | | | 18917.86 | | | 37729.91 | | | | | | 2.33E-12 | | | | | | | 11728.90 | | | | | | | |
|  | | | | TA- | | | 177.89 | | | 871.58 | | | | | | 9.52E-09 | | | | | | | 110.29 | | | | | | | |
|  | | | | Tos- | | | 288.65 | | | 746.07 | | | | | | 2.72E-08 | | | | | | | 178.96 | | | | | | | |
|  | | | | OTf- | | | 14.29 | | | 78.93 | | | | | | 4.18E-06 | | | | | | | 8.86 | | | | | | | |
|  | | | | MeSO4- | | | 105.72 | | | 448.63 | | | | | | 5.12E-08 | | | | | | | 65.55 | | | | | | | |
|  | | | | CH3OEtSO4- | | | 99.80 | | | 298.48 | | | | | | 2.32E-07 | | | | | | | 61.88 | | | | | | | |
|  | | | | PFBS- | | | 20.35 | | | 39.43 | | | | | | 6.30E-05 | | | | | | | 12.62 | | | | | | | |
|  | | | | HSO4- | | | 62.51 | | | 411.01 | | | | | | 2.32E-09 | | | | | | | 38.75 | | | | | | | |
|  | | | | H2PO4- | | | 641.11 | | | 2575.12 | | | | | | 3.85E-13 | | | | | | | 397.48 | | | | | | | |
|  | | | | Me2PO4- | | | 2266.45 | | | 5480.38 | | | | | | 1.77E-10 | | | | | | | 1405.18 | | | | | | | |
|  | | | | BF4- | | | 8.91 | | | 72.43 | | | | | | 2.91E-06 | | | | | | | 5.53 | | | | | | | |
|  | | | | ClO4- | | | 8.90 | | | 72.97 | | | | | | 3.09E-06 | | | | | | | 5.52 | | | | | | | |
|  | | | | NO3- | | | 407.07 | | | 1642.86 | | | | | | 1.80E-09 | | | | | | | 252.38 | | | | | | | |
|  | | | | SCN- | | | 92.99 | | | 522.60 | | | | | | 3.13E-08 | | | | | | | 57.65 | | | | | | | |
|  | | | | TCM- | | | 11.41 | | | 58.63 | | | | | | 9.19E-06 | | | | | | | 7.08 | | | | | | | |
|  | | | | DCA- | | | 65.12 | | | 390.00 | | | | | | 6.38E-08 | | | | | | | 40.37 | | | | | | | |
|  | | | | NTf2- | | | 3.33 | | | 4.60 | | | | | | 1.43E-02 | | | | | | | 2.06 | | | | | | | |
|  | | | | PhO- | | | 2071.19 | | | 5541.14 | | | | | | 1.52E-10 | | | | | | | 1284.12 | | | | | | | |
| PrSO3Hmim+ | | | |  | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | | | Cl- | | | 4205.09 | | | 11143.21 | | | | | | 1.50E-18 | | | | | | | 2607.12 | | | | | | | |
|  | | | | Ac- | | | 1169.50 | | | 6147.42 | | | | | | 3.80E-17 | | | | | | | 725.08 | | | | | | | |
|  | | | | TA- | | | 20.96 | | | 265.03 | | | | | | 8.35E-13 | | | | | | | 12.99 | | | | | | | |
|  | | | | Tos- | | | 58.05 | | | 331.91 | | | | | | 7.37E-13 | | | | | | | 35.99 | | | | | | | |
|  | | | | OTf- | | | 3.39 | | | 43.50 | | | | | | 1.74E-09 | | | | | | | 2.10 | | | | | | | |
|  | | | | MeSO4- | | | 17.21 | | | 248.11 | | | | | | 1.31E-12 | | | | | | | 10.67 | | | | | | | |
|  | | | | CH3OEtSO4- | | | 21.96 | | | 166.88 | | | | | | 1.04E-11 | | | | | | | 13.61 | | | | | | | |
|  | | | | PFBS- | | | 7.70 | | | 21.89 | | | | | | 7.15E-08 | | | | | | | 4.77 | | | | | | | |
|  | | HSO4- | | | | 8.37 | | | 248.58 | | | | | | 6.18E-14 | | | | | | | 5.19 | | | | | | | |
|  | | H2PO4- | | | | 78.44 | | | 1077.87 | | | | | | 5.29E-18 | | | | | | | 48.63 | | | | | | | |
|  | | Me2PO4- | | | | 279.91 | | | 1617.48 | | | | | | 2.33E-15 | | | | | | | 173.54 | | | | | | | |
|  | | BF4- | | | | 1.25 | | | 55.84 | | | | | | 1.26E-09 | | | | | | | 0.77 | | | | | | | |
|  | | ClO4- | | | | 1.29 | | | 54.08 | | | | | | 1.37E-09 | | | | | | | 0.80 | | | | | | | |
|  | | NO3- | | | | 34.04 | | | 606.46 | | | | | | 3.28E-14 | | | | | | | 21.11 | | | | | | | |
|  | | SCN- | | | | 9.20 | | | 237.47 | | | | | | 1.10E-12 | | | | | | | 5.70 | | | | | | | |
|  | | TCM- | | | | 2.89 | | | 33.88 | | | | | | 6.07E-09 | | | | | | | 1.79 | | | | | | | |
|  | | DCA- | | | | 9.07 | | | 185.38 | | | | | | 3.18E-12 | | | | | | | 5.62 | | | | | | | |
|  | | NTf2- | | | | 2.01 | | | 3.70 | | | | | | 8.17E-04 | | | | | | | 1.25 | | | | | | | |
|  | | PhO- | | | | 134.68 | | | 903.19 | | | | | | 2.88E-14 | | | | | | | 83.50 | | | | | | | |
| BPy+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 19397.04 | | | 27750.46 | | | | | | 3.42E-10 | | | | | | | 12025.98 | | | | | | | |
|  | | Ac- | | | | 24799.39 | | | 52567.11 | | | | | | 6.30E-10 | | | | | | | 15375.40 | | | | | | | |
|  | | TA- | | | | 299.95 | | | 1102.95 | | | | | | 1.16E-06 | | | | | | | 185.96 | | | | | | | |
|  | | Tos- | | | | 346.43 | | | 786.34 | | | | | | 2.00E-06 | | | | | | | 214.78 | | | | | | | |
|  | | OTf- | | | | 20.67 | | | 77.45 | | | | | | 9.81E-05 | | | | | | | 12.82 | | | | | | | |
|  | | MeSO4- | | | | 114.16 | | | 438.90 | | | | | | 2.26E-06 | | | | | | | 70.78 | | | | | | | |
|  | | CH3OEtSO4- | | | | 115.29 | | | 299.79 | | | | | | 8.54E-06 | | | | | | | 71.48 | | | | | | | |
|  | | PFBS- | | | | 27.36 | | | 41.85 | | | | | | 1.05E-03 | | | | | | | 16.96 | | | | | | | |
|  | | HSO4- | | | | 63.33 | | | 393.57 | | | | | | 9.85E-08 | | | | | | | 39.27 | | | | | | | |
|  | | H2PO4- | | | | 622.84 | | | 2732.76 | | | | | | 5.37E-11 | | | | | | | 386.16 | | | | | | | |
|  | | Me2PO4- | | | | 2604.92 | | | 6315.86 | | | | | | 3.45E-08 | | | | | | | 1615.02 | | | | | | | |
|  | | BF4- | | | | 10.29 | | | 63.35 | | | | | | 4.72E-05 | | | | | | | 6.38 | | | | | | | |
|  | | ClO4- | | | | 10.77 | | | 64.28 | | | | | | 5.42E-05 | | | | | | | 6.68 | | | | | | | |
|  | | NO3- | | | | 473.38 | | | 2001.14 | | | | | | 1.92E-07 | | | | | | | 293.49 | | | | | | | |
|  | | SCN- | | | | 117.70 | | | 585.14 | | | | | | 1.92E-06 | | | | | | | 72.97 | | | | | | | |
|  | | TCM- | | | | 16.51 | | | 57.49 | | | | | | 1.81E-04 | | | | | | | 10.24 | | | | | | | |
|  | | DCA- | | | | 85.54 | | | 394.66 | | | | | | 3.74E-06 | | | | | | | 53.03 | | | | | | | |
|  | | NTf2- | | | | 3.77 | | | 3.81 | | | | | | 6.95E-02 | | | | | | | 2.34 | | | | | | | |
|  | | PhO- | | | | 4746.64 | | | 11021.84 | | | | | | 4.26E-08 | | | | | | | 2942.87 | | | | | | | |
| BmPy+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 56503.77 | | | 57069.15 | | | | | | 1.31E-07 | | | | | | | 35031.82 | | | | | | | |
|  | | Ac- | | | | 108525.99 | | | 146225.64 | | | | | | 1.35E-07 | | | | | | | 67285.12 | | | | | | | |
|  | | TA- | | | | 941.06 | | | 1924.35 | | | | | | 3.54E-05 | | | | | | | 583.45 | | | | | | | |
|  | | Tos- | | | | 834.23 | | | 1120.93 | | | | | | 7.58E-05 | | | | | | | 517.21 | | | | | | | |
|  | | OTf- | | | | 45.63 | | | 92.40 | | | | | | 1.16E-03 | | | | | | | 28.29 | | | | | | | |
|  | | MeSO4- | | | | 291.36 | | | 552.28 | | | | | | 8.22E-05 | | | | | | | 180.64 | | | | | | | |
|  | | CH3OEtSO4- | | | | 257.66 | | | 371.23 | | | | | | 2.36E-04 | | | | | | | 159.75 | | | | | | | |
|  | | PFBS- | | | | 49.41 | | | 52.59 | | | | | | 7.79E-03 | | | | | | | 30.63 | | | | | | | |
|  | | HSO4- | | | | 169.74 | | | 478.85 | | | | | | 3.58E-06 | | | | | | | 105.24 | | | | | | | |
|  | | H2PO4- | | | | 1846.08 | | | 4380.64 | | | | | | 4.03E-09 | | | | | | | 1144.55 | | | | | | | |
|  | | Me2PO4- | | | | 8415.47 | | | 11604.60 | | | | | | 3.69E-06 | | | | | | | 5217.51 | | | | | | | |
|  | | BF4- | | | | 24.12 | | | 63.65 | | | | | | 7.01E-04 | | | | | | | 14.95 | | | | | | | |
|  | | ClO4- | | | | 25.12 | | | 65.84 | | | | | | 7.59E-04 | | | | | | | 15.58 | | | | | | | |
|  | | NO3- | | | | 1560.46 | | | 3190.23 | | | | | | 1.11E-05 | | | | | | | 967.47 | | | | | | | |
|  | | SCN- | | | | 349.04 | | | 809.72 | | | | | | 6.02E-05 | | | | | | | 216.40 | | | | | | | |
|  | | TCM- | | | | 34.87 | | | 66.82 | | | | | | 1.85E-03 | | | | | | | 21.62 | | | | | | | |
|  | | DCA- | | | | 234.96 | | | 539.56 | | | | | | 9.84E-05 | | | | | | | 145.67 | | | | | | | |
|  | | NTf2- | | | | 4.78 | | | 3.79 | | | | | | 1.71E-01 | | | | | | | 2.96 | | | | | | | |
|  | | PhO- | | | | 20043.50 | | | 28872.10 | | | | | | 2.14E-06 | | | | | | | 12426.78 | | | | | | | |
| PrSO3HPy+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 1741.01 | | | 5639.05 | | | | | | 1.82E-18 | | | | | | | 1079.41 | | | | | | | |
|  | | Ac- | | | | 605.15 | | | 4296.19 | | | | | | 8.08E-17 | | | | | | | 375.19 | | | | | | | |
|  | | TA- | | | | 14.46 | | | 236.19 | | | | | | 1.97E-12 | | | | | | | 8.97 | | | | | | | |
|  | | Tos- | | | | 34.81 | | | 267.11 | | | | | | 9.65E-13 | | | | | | | 21.58 | | | | | | | |
|  | | OTf- | | | | 2.45 | | | 39.49 | | | | | | 2.00E-09 | | | | | | | 1.52 | | | | | | | |
|  | | MeSO4- | | | | 8.71 | | | 206.26 | | | | | | 1.04E-12 | | | | | | | 5.40 | | | | | | | |
|  | | CH3OEtSO4- | | | | 12.86 | | | 141.92 | | | | | | 8.90E-12 | | | | | | | 7.97 | | | | | | | |
|  | | PFBS- | | | | 6.43 | | | 20.62 | | | | | | 1.02E-07 | | | | | | | 3.99 | | | | | | | |
|  | | HSO4- | | | | 3.83 | | | 213.79 | | | | | | 4.67E-14 | | | | | | | 2.38 | | | | | | | |
|  | | H2PO4- | | | | 38.17 | | | 874.80 | | | | | | 6.99E-18 | | | | | | | 23.67 | | | | | | | |
|  | | Me2PO4- | | | | 144.19 | | | 1190.07 | | | | | | 3.31E-15 | | | | | | | 89.40 | | | | | | | |
|  | | BF4- | | | | 0.64 | | | 51.85 | | | | | | 7.42E-10 | | | | | | | 0.40 | | | | | | | |
|  | | ClO4- | | | | 0.70 | | | 49.82 | | | | | | 9.34E-10 | | | | | | | 0.44 | | | | | | | |
|  | | NO3- | | | | 16.40 | | | 544.55 | | | | | | 3.61E-14 | | | | | | | 10.17 | | | | | | | |
|  | | SCN- | | | | 4.82 | | | 222.40 | | | | | | 1.24E-12 | | | | | | | 2.99 | | | | | | | |
|  | | TCM- | | | | 2.14 | | | 31.36 | | | | | | 6.65E-09 | | | | | | | 1.32 | | | | | | | |
|  | | DCA- | | | | 5.32 | | | 160.06 | | | | | | 4.55E-12 | | | | | | | 3.30 | | | | | | | |
|  | | NTf2- | | | | 1.91 | | | 3.60 | | | | | | 8.38E-04 | | | | | | | 1.18 | | | | | | | |
|  | | PhO- | | | | 123.12 | | | 1120.43 | | | | | | 9.49E-14 | | | | | | | 76.33 | | | | | | | |
| N1444+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 82897.14 | | | 69134.36 | | | | | | 3.67E-04 | | | | | | | 51395.47 | | | | | | | |
|  | | Ac- | | | | 433060.31 | | | 370606.32 | | | | | | 4.83E-04 | | | | | | | 268493.43 | | | | | | | |
|  | | TA- | | | | 3348.14 | | | 3076.75 | | | | | | 1.02E-02 | | | | | | | 2075.82 | | | | | | | |
|  | | Tos- | | | | 1792.83 | | | 1282.43 | | | | | | 1.67E-02 | | | | | | | 1111.54 | | | | | | | |
|  | | OTf- | | | | 103.84 | | | 87.65 | | | | | | 5.90E-02 | | | | | | | 64.38 | | | | | | | |
|  | | MeSO4- | | | | 599.74 | | | 528.70 | | | | | | 1.36E-02 | | | | | | | 371.83 | | | | | | | |
|  | | CH3OEtSO4- | | | | 503.95 | | | 365.42 | | | | | | 2.84E-02 | | | | | | | 312.45 | | | | | | | |
|  | | PFBS- | | | | 96.57 | | | 57.79 | | | | | | 2.03E-01 | | | | | | | 59.87 | | | | | | | |
|  | | HSO4- | | | | 364.50 | | | 435.73 | | | | | | 6.48E-04 | | | | | | | 225.99 | | | | | | | |
|  | | H2PO4- | | | | 4318.02 | | | 5410.83 | | | | | | 2.54E-06 | | | | | | | 2677.13 | | | | | | | |
|  | | Me2PO4- | | | | 21974.57 | | | 16972.91 | | | | | | 3.34E-03 | | | | | | | 13624.03 | | | | | | | |
|  | | BF4- | | | | 47.45 | | | 47.13 | | | | | | 3.56E-02 | | | | | | | 29.42 | | | | | | | |
|  | | ClO4- | | | | 50.89 | | | 49.99 | | | | | | 3.83E-02 | | | | | | | 31.55 | | | | | | | |
|  | | NO3- | | | | 4315.49 | | | 4311.22 | | | | | | 4.53E-03 | | | | | | | 2675.56 | | | | | | | |
|  | | SCN- | | | | 918.27 | | | 919.63 | | | | | | 1.12E-02 | | | | | | | 569.32 | | | | | | | |
|  | | TCM- | | | | 77.58 | | | 62.59 | | | | | | 7.74E-02 | | | | | | | 48.10 | | | | | | | |
|  | | DCA- | | | | 596.82 | | | 571.60 | | | | | | 1.58E-02 | | | | | | | 370.02 | | | | | | | |
|  | | NTf2- | | | | 6.36 | | | 3.14 | | | | | | 9.16E-01 | | | | | | | 3.94 | | | | | | | |
|  | | PhO- | | | | 100433.43 | | | 80281.26 | | | | | | 2.66E-03 | | | | | | | 62267.81 | | | | | | | |
| N122,1O2+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 137968.55 | | | 59153.19 | | | | | | 1.09E-06 | | | | | | | 85539.24 | | | | | | | |
|  | | Ac- | | | | 231502.69 | | | 222374.35 | | | | | | 1.13E-06 | | | | | | | 143529.55 | | | | | | | |
|  | | TA- | | | | 1233.29 | | | 3034.00 | | | | | | 6.61E-05 | | | | | | | 764.63 | | | | | | | |
|  | | Tos- | | | | 941.04 | | | 1383.44 | | | | | | 1.24E-04 | | | | | | | 583.43 | | | | | | | |
|  | | OTf- | | | | 45.80 | | | 128.07 | | | | | | 7.88E-04 | | | | | | | 28.40 | | | | | | | |
|  | | MeSO4- | | | | 376.40 | | | 690.94 | | | | | | 9.63E-05 | | | | | | | 233.36 | | | | | | | |
|  | | CH3OEtSO4- | | | | 292.92 | | | 455.01 | | | | | | 2.61E-04 | | | | | | | 181.61 | | | | | | | |
|  | | PFBS- | | | | 52.57 | | | 68.43 | | | | | | 7.16E-03 | | | | | | | 32.59 | | | | | | | |
|  | | HSO4- | | | | 254.87 | | | 616.28 | | | | | | 3.77E-06 | | | | | | | 158.02 | | | | | | | |
|  | | H2PO4- | | | | 3422.60 | | | 5661.19 | | | | | | 1.08E-08 | | | | | | | 2121.98 | | | | | | | |
|  | | Me2PO4- | | | | 11508.84 | | | 14503.55 | | | | | | 1.30E-05 | | | | | | | 7135.37 | | | | | | | |
|  | | BF4- | | | | 30.48 | | | 87.02 | | | | | | 3.44E-04 | | | | | | | 18.90 | | | | | | | |
|  | | ClO4- | | | | 30.50 | | | 90.92 | | | | | | 3.77E-04 | | | | | | | 18.91 | | | | | | | |
|  | | NO3- | | | | 2958.10 | | | 4536.97 | | | | | | 2.26E-05 | | | | | | | 1833.99 | | | | | | | |
|  | | SCN- | | | | 533.97 | | | 1159.35 | | | | | | 7.25E-05 | | | | | | | 331.06 | | | | | | | |
|  | | TCM- | | | | 35.45 | | | 92.76 | | | | | | 1.17E-03 | | | | | | | 21.98 | | | | | | | |
|  | | DCA- | | | | 289.98 | | | 747.69 | | | | | | 1.15E-04 | | | | | | | 179.79 | | | | | | | |
|  | | NTf2- | | | | 5.00 | | | 5.34 | | | | | | 7.11E-02 | | | | | | | 3.10 | | | | | | | |
|  | | PhO- | | | | 33065.90 | | | 50113.00 | | | | | | 1.08E-05 | | | | | | | 20500.56 | | | | | | | |
| P1444+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 106068.02 | | | 76069.20 | | | | | | 3.09E-03 | | | | | | | 65761.20 | | | | | | | |
|  | | Ac- | | | | 706887.17 | | | 514447.82 | | | | | | 4.09E-03 | | | | | | | 438263.58 | | | | | | | |
|  | | TA- | | | | 4843.84 | | | 3671.96 | | | | | | 4.03E-02 | | | | | | | 3003.13 | | | | | | | |
|  | | Tos- | | | | 2266.54 | | | 1371.36 | | | | | | 6.38E-02 | | | | | | | 1405.23 | | | | | | | |
|  | | OTf- | | | | 127.04 | | | 88.58 | | | | | | 1.49E-01 | | | | | | | 78.77 | | | | | | | |
|  | | MeSO4- | | | | 743.26 | | | 538.86 | | | | | | 4.80E-02 | | | | | | | 460.81 | | | | | | | |
|  | | CH3OEtSO4- | | | | 611.47 | | | 373.00 | | | | | | 9.21E-02 | | | | | | | 379.10 | | | | | | | |
|  | | PFBS- | | | | 116.07 | | | 60.17 | | | | | | 4.53E-01 | | | | | | | 71.96 | | | | | | | |
|  | | HSO4- | | | | 456.23 | | | 439.09 | | | | | | 2.29E-03 | | | | | | | 282.86 | | | | | | | |
|  | | H2PO4- | | | | 5789.10 | | | 5974.49 | | | | | | 1.27E-05 | | | | | | | 3589.19 | | | | | | | |
|  | | Me2PO4- | | | | 30167.18 | | | 19641.14 | | | | | | 1.89E-02 | | | | | | | 18703.37 | | | | | | | |
|  | | BF4- | | | | 55.77 | | | 44.75 | | | | | | 8.96E-02 | | | | | | | 34.58 | | | | | | | |
|  | | ClO4- | | | | 60.11 | | | 47.79 | | | | | | 9.56E-02 | | | | | | | 37.27 | | | | | | | |
|  | | NO3- | | | | 5978.53 | | | 4885.56 | | | | | | 2.00E-02 | | | | | | | 3706.63 | | | | | | | |
|  | | SCN- | | | | 1214.99 | | | 988.28 | | | | | | 3.93E-02 | | | | | | | 753.28 | | | | | | | |
|  | | TCM- | | | | 93.62 | | | 62.85 | | | | | | 1.84E-01 | | | | | | | 58.05 | | | | | | | |
|  | | DCA- | | | | 770.96 | | | 602.08 | | | | | | 5.31E-02 | | | | | | | 477.99 | | | | | | | |
|  | | NTf2- | | | | 6.74 | | | 3.00 | | | | | | 1.37E+00 | | | | | | | 4.18 | | | | | | | |
|  | | PhO- | | | | 166131.48 | | | 113147.05 | | | | | | 1.59E-02 | | | | | | | 103000.00 | | | | | | | |
| P4446+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 103200.22 | | | 65626.22 | | | | | | 1.28E-02 | | | | | | | 63983.19 | | | | | | | |
|  | | Ac- | | | | 794958.07 | | | 477130.19 | | | | | | 1.72E-02 | | | | | | | 492866.74 | | | | | | | |
|  | | TA- | | | | 5604.26 | | | 3098.38 | | | | | | 1.58E-01 | | | | | | | 3474.59 | | | | | | | |
|  | | Tos- | | | | 2461.87 | | | 1145.90 | | | | | | 2.54E-01 | | | | | | | 1526.34 | | | | | | | |
|  | | OTf- | | | | 139.17 | | | 69.02 | | | | | | 5.34E-01 | | | | | | | 86.28 | | | | | | | |
|  | | MeSO4- | | | | 793.98 | | | 421.91 | | | | | | 2.06E-01 | | | | | | | 492.26 | | | | | | | |
|  | | CH3OEtSO4- | | | | 651.22 | | | 299.69 | | | | | | 3.73E-01 | | | | | | | 403.75 | | | | | | | |
|  | | PFBS- | | | | 122.32 | | | 50.24 | | | | | | 1.20E+00 | | | | | | | 75.84 | | | | | | | |
|  | | HSO4- | | | | 501.43 | | | 334.43 | | | | | | 1.14E-02 | | | | | | | 310.88 | | | | | | | |
|  | | H2PO4- | | | | 6367.62 | | | 4877.41 | | | | | | 6.46E-05 | | | | | | | 3947.87 | | | | | | | |
|  | | Me2PO4- | | | | 33283.32 | | | 17096.45 | | | | | | 7.97E-02 | | | | | | | 20635.35 | | | | | | | |
|  | | BF4- | | | | 59.35 | | | 32.23 | | | | | | 3.86E-01 | | | | | | | 36.80 | | | | | | | |
|  | | ClO4- | | | | 64.46 | | | 34.67 | | | | | | 4.06E-01 | | | | | | | 39.96 | | | | | | | |
|  | | NO3- | | | | 6558.65 | | | 3942.38 | | | | | | 9.00E-02 | | | | | | | 4066.30 | | | | | | | |
|  | | SCN- | | | | 1342.46 | | | 772.92 | | | | | | 1.72E-01 | | | | | | | 832.31 | | | | | | | |
|  | | TCM- | | | | 102.24 | | | 48.89 | | | | | | 6.58E-01 | | | | | | | 63.39 | | | | | | | |
|  | | DCA- | | | | 858.18 | | | 474.88 | | | | | | 2.19E-01 | | | | | | | 532.06 | | | | | | | |
|  | | NTf2- | | | | 6.67 | | | 2.39 | | | | | | 3.16E+00 | | | | | | | 4.14 | | | | | | | |
|  | | PhO- | | | | 192877.87 | | | 102185.79 | | | | | | 6.39E-02 | | | | | | | 119582.52 | | | | | | | |
| P14+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 162287.39 | | | 75975.96 | | | | | | 5.11E-05 | | | | | | | 100616.70 | | | | | | | |
|  | | Ac- | | | | 448890.09 | | | 395182.26 | | | | | | 5.56E-05 | | | | | | | 278307.75 | | | | | | | |
|  | | TA- | | | | 2313.00 | | | 4072.08 | | | | | | 1.00E-03 | | | | | | | 1434.04 | | | | | | | |
|  | | Tos- | | | | 1422.88 | | | 1624.93 | | | | | | 1.70E-03 | | | | | | | 882.17 | | | | | | | |
|  | | OTf- | | | | 70.66 | | | 131.72 | | | | | | 5.53E-03 | | | | | | | 43.81 | | | | | | | |
|  | | MeSO4- | | | | 530.60 | | | 754.91 | | | | | | 1.17E-03 | | | | | | | 328.97 | | | | | | | |
|  | | CH3OEtSO4- | | | | 416.21 | | | 495.65 | | | | | | 2.71E-03 | | | | | | | 258.05 | | | | | | | |
|  | | PFBS- | | | | 75.08 | | | 73.95 | | | | | | 3.76E-02 | | | | | | | 46.55 | | | | | | | |
|  | | HSO4- | | | | 339.54 | | | 661.93 | | | | | | 4.49E-05 | | | | | | | 210.51 | | | | | | | |
|  | | H2PO4- | | | | 4723.40 | | | 7078.63 | | | | | | 2.10E-07 | | | | | | | 2928.47 | | | | | | | |
|  | | Me2PO4- | | | | 18804.09 | | | 19643.32 | | | | | | 3.34E-04 | | | | | | | 11658.36 | | | | | | | |
|  | | BF4- | | | | 39.58 | | | 81.78 | | | | | | 2.59E-03 | | | | | | | 24.54 | | | | | | | |
|  | | ClO4- | | | | 40.81 | | | 85.99 | | | | | | 2.85E-03 | | | | | | | 25.30 | | | | | | | |
|  | | NO3- | | | | 4495.52 | | | 5923.62 | | | | | | 3.93E-04 | | | | | | | 2787.18 | | | | | | | |
|  | | SCN- | | | | 806.37 | | | 1445.36 | | | | | | 9.06E-04 | | | | | | | 499.94 | | | | | | | |
|  | | TCM- | | | | 53.40 | | | 93.99 | | | | | | 7.87E-03 | | | | | | | 33.11 | | | | | | | |
|  | | DCA- | | | | 451.10 | | | 838.47 | | | | | | 1.35E-03 | | | | | | | 279.68 | | | | | | | |
|  | | NTf2- | | | | 5.39 | | | 4.39 | | | | | | 2.06E-01 | | | | | | | 3.34 | | | | | | | |
|  | | PhO- | | | | 75074.82 | | | 91205.04 | | | | | | 3.04E-04 | | | | | | | 46545.70 | | | | | | | |
| PP14+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 142777.76 | | | 79831.67 | | | | | | 8.25E-05 | | | | | | | 88520.91 | | | | | | | |
|  | | Ac- | | | | 466149.93 | | | 410705.92 | | | | | | 9.16E-05 | | | | | | | 289008.70 | | | | | | | |
|  | | TA- | | | | 2655.64 | | | 3990.08 | | | | | | 1.66E-03 | | | | | | | 1646.47 | | | | | | | |
|  | | Tos- | | | | 1574.24 | | | 1603.40 | | | | | | 2.84E-03 | | | | | | | 976.01 | | | | | | | |
|  | | OTf- | | | | 80.87 | | | 124.49 | | | | | | 9.73E-03 | | | | | | | 50.14 | | | | | | | |
|  | | MeSO4- | | | | 574.70 | | | 727.70 | | | | | | 2.08E-03 | | | | | | | 356.31 | | | | | | | |
|  | | CH3OEtSO4- | | | | 457.46 | | | 481.24 | | | | | | 4.69E-03 | | | | | | | 283.62 | | | | | | | |
|  | | PFBS- | | | | 81.27 | | | 72.17 | | | | | | 5.25E-02 | | | | | | | 50.38 | | | | | | | |
|  | | HSO4- | | | | 358.67 | | | 628.73 | | | | | | 8.29E-05 | | | | | | | 222.37 | | | | | | | |
|  | | H2PO4- | | | | 4775.87 | | | 6992.62 | | | | | | 3.64E-07 | | | | | | | 2961.00 | | | | | | | |
|  | | Me2PO4- | | | | 20648.49 | | | 20010.39 | | | | | | 5.74E-04 | | | | | | | 12801.87 | | | | | | | |
|  | | BF4- | | | | 43.38 | | | 75.08 | | | | | | 4.76E-03 | | | | | | | 26.89 | | | | | | | |
|  | | ClO4- | | | | 45.03 | | | 79.08 | | | | | | 5.15E-03 | | | | | | | 27.92 | | | | | | | |
|  | | NO3- | | | | 4642.16 | | | 5787.97 | | | | | | 6.96E-04 | | | | | | | 2878.10 | | | | | | | |
|  | | SCN- | | | | 870.42 | | | 1304.35 | | | | | | 1.62E-03 | | | | | | | 539.66 | | | | | | | |
|  | | TCM- | | | | 60.95 | | | 88.88 | | | | | | 1.31E-02 | | | | | | | 37.79 | | | | | | | |
|  | | DCA- | | | | 507.20 | | | 801.99 | | | | | | 2.36E-03 | | | | | | | 314.46 | | | | | | | |
|  | | NTf2- | | | | 5.68 | | | 4.18 | | | | | | 2.74E-01 | | | | | | | 3.52 | | | | | | | |
|  | | PhO- | | | | 84691.10 | | | 92990.21 | | | | | | 4.79E-04 | | | | | | | 52507.71 | | | | | | | |
| BmMor+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 47302.43 | | | 34303.38 | | | | | | 1.14E-08 | | | | | | | 29327.07 | | | | | | | |
|  | | Ac- | | | | 63944.66 | | | 97984.86 | | | | | | 1.92E-08 | | | | | | | 39645.10 | | | | | | | |
|  | | TA- | | | | 483.58 | | | 1791.87 | | | | | | 6.09E-06 | | | | | | | 299.81 | | | | | | | |
|  | | Tos- | | | | 453.72 | | | 973.64 | | | | | | 9.37E-06 | | | | | | | 281.30 | | | | | | | |
|  | | OTf- | | | | 24.84 | | | 99.48 | | | | | | 1.58E-04 | | | | | | | 15.40 | | | | | | | |
|  | | MeSO4- | | | | 160.21 | | | 526.92 | | | | | | 7.24E-06 | | | | | | | 99.33 | | | | | | | |
|  | | CH3OEtSO4- | | | | 145.76 | | | 352.88 | | | | | | 2.45E-05 | | | | | | | 90.37 | | | | | | | |
|  | | PFBS- | | | | 34.50 | | | 53.45 | | | | | | 1.96E-03 | | | | | | | 21.39 | | | | | | | |
|  | | HSO4- | | | | 98.57 | | | 483.27 | | | | | | 2.88E-07 | | | | | | | 61.11 | | | | | | | |
|  | | H2PO4- | | | | 1223.65 | | | 3736.75 | | | | | | 4.53E-10 | | | | | | | 758.65 | | | | | | | |
|  | | Me2PO4- | | | | 4297.57 | | | 8521.76 | | | | | | 4.15E-07 | | | | | | | 2664.46 | | | | | | | |
|  | | BF4- | | | | 13.15 | | | 76.74 | | | | | | 5.26E-05 | | | | | | | 8.15 | | | | | | | |
|  | | ClO4- | | | | 13.45 | | | 78.89 | | | | | | 6.14E-05 | | | | | | | 8.34 | | | | | | | |
|  | | NO3- | | | | 939.68 | | | 2919.87 | | | | | | 1.12E-06 | | | | | | | 582.59 | | | | | | | |
|  | | SCN- | | | | 190.80 | | | 819.01 | | | | | | 6.04E-06 | | | | | | | 118.29 | | | | | | | |
|  | | TCM- | | | | 19.89 | | | 73.65 | | | | | | 2.61E-04 | | | | | | | 12.33 | | | | | | | |
|  | | DCA- | | | | 120.57 | | | 532.52 | | | | | | 1.18E-05 | | | | | | | 74.75 | | | | | | | |
|  | | NTf2- | | | | 4.36 | | | 5.00 | | | | | | 4.38E-02 | | | | | | | 2.71 | | | | | | | |
|  | | PhO- | | | | 9989.41 | | | 22213.86 | | | | | | 5.70E-07 | | | | | | | 6193.34 | | | | | | | |
| Tmgh+ | |  | | | |  | | |  | | | | | |  | | | | | | |  | | | | | | | |
|  | | Cl- | | | | 500649.40 | | | 81199.88 | | | | | | 2.23E-07 | | | | | | | 310398.05 | | | | | | | |
|  | | Ac- | | | | 353366.58 | | | 231686.20 | | | | | | 1.09E-07 | | | | | | | 219084.05 | | | | | | | |
|  | | TA- | | | | 1166.05 | | | 3365.98 | | | | | | 7.17E-06 | | | | | | | 722.94 | | | | | | | |
|  | Tos- | | | | | | | 1052.27 | | | | | | 1646.51 | | | | | | | 2.12E-05 | | | | | | | 652.40 | |
|  | | | OTf- | | | | 39.15 | | | | | 151.37 | | | | | | | 2.02E-04 | | | | | | | 24.27 | | | |
|  | | | MeSO4- | | | | 492.62 | | | | | 848.69 | | | | | | | 2.25E-05 | | | | | | | 305.42 | | | |
|  | | | CH3OEtSO4- | | | | 325.85 | | | | | 538.02 | | | | | | | 6.24E-05 | | | | | | | 202.03 | | | |
|  | | | PFBS- | | | | 46.02 | | | | | 71.77 | | | | | | | 2.14E-03 | | | | | | | 28.53 | | | |
|  | | | HSO4- | | | | 387.42 | | | | | 759.80 | | | | | | | 8.68E-07 | | | | | | | 240.20 | | | |
|  | | | H2PO4- | | | | 6185.61 | | | | | 6899.46 | | | | | | | 1.45E-09 | | | | | | | 3835.02 | | | |
|  | | | Me2PO4- | | | | 15499.39 | | | | | 17528.83 | | | | | | | 1.52E-06 | | | | | | | 9609.48 | | | |
|  | | | BF4- | | | | 37.52 | | | | | 107.88 | | | | | | | 1.21E-04 | | | | | | | 23.26 | | | |
|  | | | ClO4- | | | | 35.46 | | | | | 113.02 | | | | | | | 1.24E-04 | | | | | | | 21.99 | | | |
|  | | NO3- | | | | | 4984.07 | | | | | | 5083.22 | | | | | 3.45E-06 | | | | | | | 3090.08 | | | | |
|  | | SCN- | | | | | 736.65 | | | | | | 1353.70 | | | | | | | 1.29E-05 | | | | | | | 456.72 | |
|  | | TCM- | | | | | 29.57 | | | | | | 107.23 | | | | | | | 3.24E-04 | | | | | | | 18.33 | |
|  | | DCA- | | | | | 333.81 | | | | | | 935.70 | | | | | 2.01E-05 | | | | | | | | 206.96 | | | | | | |
|  | | NTf2- | | | | | 3.89 | | | | | | 5.07 | | | | | 4.60E-02 | | | | | | | | 2.41 | | | | | | |
|  | | PhO- | | | | | 39368.98 | | | | | | 60056.14 | | | | | 5.42E-07 | | | | | | | | 24408.41 | | | | | | |