

## List of bands observed in Fourier-transform infrared and Fourier-transform Raman spectra observed in the title structures

### Abbreviations and symbols:

vs, very strong; s, strong; m, medium; w, weak; vw, very weak; b, broad; sh, shoulder.

### **2-athdox** (2-amino-1,3,4-thiadiazolium(1+) hydrogen oxalate):

**FTIR spectrum:**  $\nu_{\max}/\text{cm}^{-1}$  3246mb, 3117m, 3055mb, 2896mb, 2748m, 2714mb, 2351wb, 2229w, 2049wb, 1759m, 1663m, 1652m, 1644w, 1592w, 1558w, 1535m, 1515wb, 1409m, 1336sh, 1316m, 1231m, 1174m, 1117m, 1062m, 992w, 900m, 866m, 842sh, 791m, 744w, 729vs, 707m, 631m, 607m, 575m, 555sh, 536m, 481m, 459m, 399m, 319m, 244w, 165m, 139m, 126m, 94w, 59w.

**FT Raman spectrum:**  $\nu_{\max}/\text{cm}^{-1}$  3117m, 3292m, 1760m, 1686w, 1662w, 1640w, 1592wb, 1531m, 1502m, 1442m, 1418s, 1373mb, 1252m, 1230s, 1218m, 1145s, 1115m, 1063m, 889s, 870s, 844m, 767s, 754vs, 728w, 711s, 680m, 628w, 576s, 537m, 458s, 397s, 309w, 262w, 248w, 178w.

### **2-athdsuc** (2-amino-1,3,4-thiadiazole bis(succinic acid)):

**FTIR spectrum:**  $\nu_{\max}/\text{cm}^{-1}$  3358m, 3309m, 3200m, 3157sh, 3112m, 2726mb, 2589mb, 2522mb, 1851mb, 1713m, 1639m, 1560w, 1516m, 1478w, 1469w, 1434w, 1420m, 1370m, 1320m, 1212w, 1179m, 1126w, 1074w, 1031m, 954w, 909m, 901w, 832m, 801m, 783w, 695m, 637m, 586m, 554m, 538m, 513m, 400m, 279w, 218m, 201m, 144m, 130m, 117w.

**FT Raman spectrum:**  $\nu_{\max}/\text{cm}^{-1}$  3309w, 3206m, 3112s, 2953s, 2931s, 2917s, 2823w, 2557w, 1709s, 1699m, 1640m, 1559w, 1515s, 1468s, 1442w, 1420s, 1392w, 1347m, 1299m, 1281m, 1258m, 1216s, 1124mb, 1075m, 1028m, 939s, 930s, 906m, 833w, 781vs, 754w, 695vs, 586m, 526w, 401vs, 284s, 274m, 264m, 179wb, 146wb.

### **2-athdglut** (2-amino-1,3,4-thiadiazole glutaric acid):

**FTIR spectrum:**  $\nu_{\max}/\text{cm}^{-1}$  3383m, 3270m, 3183m, 3095m, 2969m, 2951m, 2940m, 2909m, 2895m, 2842m, 2749m, 2572mb, 1823wb, 1766w, 1724s, 1694m, 1615m, 1515s, 1484w, 1460m, 1438sh, 1420w, 1394vs, 1370s, 1288vs, 1235m, 1225m, 1185vs, 1157w, 1068m, 1039s, 953mb, 912s, 884m, 853w, 819w, 809m, 781w, 751m, 703m, 686w, 653m, 632w, 586w, 585w, 573w, 560w, 550w, 495m, 463s, 399s, 266s, 196w, 159w, 139m, 120w, 101w.

**FT Raman spectrum:**  $\nu_{\max}/\text{cm}^{-1}$  3298w, 3167m, 3083s, 2928s, 2918vs, 2907vs, 2882m, 1712s, 1639m, 1519s, 1491w, 1459s, 1444m, 1416m, 1408m, 1362m, 1306m, 1247m, 1232s, 1186w, 1140m, 1079m, 1054m, 1036m, 919m, 906s, 822w, 787vs, 744w, 704s, 665m, 628w, 586m, 557w, 520m, 416s, 358w, 291m, 274m, 227w, 199m.

### **2-athdadip** (2-amino-1,3,4-thiadiazole adipic acid):

**FTIR spectrum:**  $\nu_{\max}/\text{cm}^{-1}$  3342m, 3286m, 3169m, 3083m, 2992m, 2953m, 2908w, 2881m, 2836wb, 2767wb, 2574mb, 2541mb, 1802wb, 1714m, 1697m, 1637m, 1578vw, 1571vw, 1560vw, 1522s, 1492sh, 1468m, 1459m, 1409s, 1389sh, 1375vs, 1277vs, 1220w, 1188vs, 1144vw, 1081vw, 1037m, 916mb, 897sh, 825m, 796vw, 786vw, 743m, 704m, 678m, 665m, 585m, 559mb, 532sh, 519m, 503m, 416s, 357m, 289m, 273w, 233w, 228wb, 200mb, 147sh, 125sh, 101w.

**FT Raman spectrum:**  $\nu_{\max}/\text{cm}^{-1}$  3377w, 3272w, 3184w, 3095s, 2969sh, 2933s, 2920s, 2910s, 2892m, 1764vw, 1722s, 1696m, 1614m, 1515m, 1459s, 1418m, 1399m, 1364m, 1293m, 1283m, 1233s, 1186w, 1134m, 1069m, 1054m, 1039m, 936s, 911m, 883w, 856w, 780vs, 756w, 700s, 686m, 652w, 587m, 555w, 462m, 401s, 287m, 266m, 190mb.