Supplemental Material

Peak identification in the mass spectrum in Figure2:

|  |  |  |
| --- | --- | --- |
| Peak position / amu | Compound  | Charge state |
| 1 | H | 1+ |
| 2 | H2 | 1+ |
| 12 | C | 1+ |
| 16 | O | 1+ |
| 17 | OH | 1+ |
| 18 | OH2 | 1+ |
| 28 | N2 | 1+ |
| 29, 30, 30.5, 31, 32 | Ni | 2+ |
| 38, 39, 39.5, 40, 41 | NiOH2 | 2+ |
| 58, 60, 61, 62, 64 | Ni | 1+ |
| 63, 65 | Cu | 1+ |

Diffusion controlled samples:

623 K:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| No. | t/h | lnD | d(lnD) | D |
| 1 | 168 | -54.11 | 1.04E-03 | 3.17E-24 |
| 2 | 168 | -54.43 | 1.22E-01 | 2.31E-24 |
| 3 | 168 | -53.49 | 3.41E-01 | 5.86E-24 |
| 4 | 168 | -53.87 | 4.16E-02 | 4.01E-24 |
| 5 | 336 | -53.77 | 9.66E-02 | 4.46E-24 |
| 6 | 336 | -54.40 | 1.05E-01 | 2.36E-24 |
| 7 | 336 | -54.19 | 1.30E-02 | 2.92E-24 |
| 8 | 336 | -54.37 | 8.66E-02 | 2.44E-24 |
| 9 | 336 | -53.98 | 9.04E-03 | 3.60E-24 |
| 10 | 336 | -54.16 | 6.34E-03 | 3.02E-24 |
| 11 | 384 | -53.96 | 8.66E-01 | 3.69E-24 |
| 12 | 384 | -54.00 | 7.93E-01 | 3.54E-24 |
| 13 | 384 | -54.49 | 1.55E-01 | 2.16E-24 |
| 14 | 384 | -54.94 | 2.83E-03 | 1.38E-24 |
| 15 | 384 | -55.55 | 4.32E-01 | 7.54E-25 |
| 16 | 384 | -55.84 | 9.00E-01 | 5.63E-25 |
| 17 | 384 | -55.11 | 5.05E-02 | 1.16E-24 |
| 18 | 384 | -54.02 | 7.49E-01 | 3.45E-24 |
| 19 | 384 | -54.18 | 5.00E-01 | 2.95E-24 |
| 20 | 384 | -54.42 | 2.15E-01 | 2.31E-24 |
| 21 | 384 | -54.56 | 1.08E-01 | 2.02E-24 |
| 22 | 384 | -54.44 | 2.03E-01 | 2.28E-24 |
| 23 | 720 | -56.04 | 1.32E+00 | 4.60E-25 |
| 24 | 720 | -56.63 | 3.05E+00 | 2.54E-25 |
| 25 | 720 | -56.51 | 2.62E+00 | 2.88E-25 |
| 26 | 720 | -56.66 | 3.13E+00 | 2.48E-25 |
| 27 | 720 | -56.00 | 1.24E+00 | 4.78E-25 |
| 28 | 720 | -56.02 | 1.28E+00 | 4.69E-25 |
| 29 | 720 | -56.15 | 1.59E+00 | 4.12E-25 |
| 30 | 720 | -55.89 | 1.01E+00 | 5.32E-25 |
| 31 | 720 | -55.69 | 6.38E-01 | 6.54E-25 |
| 32 | 720 | -55.24 | 1.21E-01 | 1.03E-24 |
| 33 | 720 | -55.41 | 2.69E-01 | 8.65E-25 |
| 34 | 1056 | -55.06 | 3.13E-02 | 1.22E-24 |
| 35 | 1056 | -55.66 | 5.90E-01 | 6.75E-25 |
| 36 | 1056 | -55.46 | 3.29E-01 | 8.20E-25 |
| 37 | 1056 | -54.46 | 1.81E-01 | 2.22E-24 |
| 38 | 1056 | -54.47 | 1.75E-01 | 2.21E-24 |
| 39 | 1056 | -54.37 | 2.63E-01 | 2.43E-24 |
| 40 | 1056 | -54.34 | 3.00E-01 | 2.52E-24 |
| 41 | 1056 | -55.48 | 3.57E-01 | 8.00E-25 |
| 42 | 1056 | -55.31 | 1.76E-01 | 9.56E-25 |
| 43 | 1056 | -55.01 | 1.59E-02 | 1.28E-24 |
| 44 | 1440 | -55.10 | 4.65E-02 | 1.17E-24 |
| 45 | 1440 | -54.73 | 2.49E-02 | 1.70E-24 |
| 46 | 1440 | -54.51 | 1.44E-01 | 2.12E-24 |
| 47 | 1440 | -54.68 | 4.37E-02 | 1.79E-24 |
| 48 | 1440 | -54.95 | 4.38E-03 | 1.36E-24 |
| 49 | 1440 | -53.50 | 1.91E+00 | 5.80E-24 |
| 50 | 1440 | -53.91 | 9.55E-01 | 3.86E-24 |
| 51 | 1440 | -55.19 | 9.16E-02 | 1.07E-24 |
| 52 | 1440 | -55.28 | 1.56E-01 | 9.80E-25 |
| 53 | 1440 | -54.67 | 4.65E-02 | 1.80E-24 |
| 54 | 1440 | -55.26 | 1.39E-01 | 1.00E-24 |
|  | Sum | -5.49E+01 |  | 1.92E-24 |
|  | Error |  | 0.098 | 1.42E-25 |

673 K:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| No. | t/h | lnD | d(lnD) | D(673K) |
| 1 | 24 | -50.97 | 8.39E-01 | 7.29E-23 |
| 2 | 24 | -50.99 | 8.02E-01 | 7.14E-23 |
| 3 | 24 | -50.86 | 1.05E+00 | 8.14E-23 |
| 4 | 24 | -50.81 | 1.16E+00 | 8.55E-23 |
| 5 | 24 | -51.00 | 7.97E-01 | 7.12E-23 |
| 6 | 24 | -51.27 | 3.79E-01 | 5.39E-23 |
| 7 | 24 | -51.24 | 4.20E-01 | 5.57E-23 |
| 8 | 60 | -51.19 | 4.88E-01 | 5.86E-23 |
| 9 | 60 | -50.94 | 9.07E-01 | 7.56E-23 |
| 10 | 60 | -50.92 | 9.37E-01 | 7.67E-23 |
| 11 | 60 | -51.81 | 7.11E-03 | 3.17E-23 |
| 12 | 60 | -52.10 | 4.43E-02 | 2.36E-23 |
| 13 | 60 | -52.22 | 1.06E-01 | 2.10E-23 |
| 14 | 60 | -52.69 | 6.48E-01 | 1.30E-23 |
| 15 | 60 | -52.35 | 2.16E-01 | 1.83E-23 |
| 16 | 60 | -51.52 | 1.39E-01 | 4.23E-23 |
| 17 | 60 | -51.53 | 1.26E-01 | 4.16E-23 |
| 18 | 60 | -51.87 | 2.36E-04 | 2.96E-23 |
| 19 | 108 | -51.62 | 7.28E-02 | 3.82E-23 |
| 20 | 108 | -51.96 | 5.40E-03 | 2.71E-23 |
| 21 | 108 | -52.70 | 6.64E-01 | 1.29E-23 |
| 22 | 108 | -52.79 | 8.05E-01 | 1.19E-23 |
| 23 | 108 | -52.75 | 7.41E-01 | 1.23E-23 |
| 24 | 108 | -52.57 | 4.69E-01 | 1.47E-23 |
| 25 | 108 | -52.84 | 8.95E-01 | 1.13E-23 |
| 26 | 168 | -51.64 | 6.16E-02 | 3.74E-23 |
| 27 | 168 | -52.04 | 2.15E-02 | 2.52E-23 |
| 28 | 168 | -51.54 | 1.23E-01 | 4.14E-23 |
| 29 | 168 | -51.85 | 1.79E-03 | 3.04E-23 |
| 30 | 168 | -51.73 | 2.42E-02 | 3.41E-23 |
| 31 | 168 | -51.95 | 3.59E-03 | 2.75E-23 |
| 32 | 168 | -52.09 | 3.98E-02 | 2.39E-23 |
| 33 | 168 | -52.37 | 2.35E-01 | 1.80E-23 |
| 34 | 168 | -52.33 | 1.91E-01 | 1.88E-23 |
| 35 | 264 | -52.09 | 3.92E-02 | 2.39E-23 |
| 36 | 264 | -52.69 | 6.35E-01 | 1.31E-23 |
| 37 | 264 | -51.02 | 7.58E-01 | 6.96E-23 |
| 38 | 264 | -51.30 | 3.43E-01 | 5.23E-23 |
| 39 | 264 | -51.88 | 2.74E-05 | 2.93E-23 |
| 40 | 264 | -51.52 | 1.37E-01 | 4.22E-23 |
| 41 | 336 | -52.39 | 2.49E-01 | 1.77E-23 |
| 42 | 336 | -52.76 | 7.60E-01 | 1.22E-23 |
| 43 | 336 | -52.94 | 1.10E+00 | 1.02E-23 |
| 44 | 336 | -53.27 | 1.89E+00 | 7.36E-24 |
| 45 | 336 | -52.10 | 4.37E-02 | 2.37E-23 |
|  | Sum | -51.89 |  | 3.58E-23 |
|  | Error |  | 0.10 | 2.88E-24 |

Determination of the phase boundary at 573 K:

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No.  | t/h | sample | Cu | dCu | Ni | dNi | k | d |
| 1 | 458 | A11\_1 | 0.7726 | 0.0009 | 0.3587 | 0.0002 | 2.0725 | 14.8369 |
| 2 |  | A11\_2 | 0.7663 | 0.0006 | 0.3342 | 0.0001 | 2.1210 | 17.1384 |
| 3 |  | A11\_3 | 0.7802 | 0.0014 | 0.3454 | 0.0000 | 2.3219 | 16.2001 |
| 4 |  | A11\_4 | 0.7160 | 0.0007 | 0.3193 | 0.0006 | 1.4369 | 14.8566 |
| 5 |  | A8\_1 | 0.7313 | 0.0001 | 0.3138 | 0.0009 | 1.7879 | 11.8508 |
| 6 |  | A8\_2 | 0.7357 | 0.0000 | 0.3131 | 0.0010 | 1.5389 | 12.9765 |
| 7 |  | A8\_3 | 0.7507 | 0.0001 | 0.3210 | 0.0005 | 1.7597 | 12.7249 |
| 8 |  | A8\_4 | 0.7315 | 0.0001 | 0.3347 | 0.0001 | 2.5406 | 12.1219 |
| 9 |  | A8\_5 | 0.7274 | 0.0002 | 0.3456 | 0.0000 | 1.3396 | 12.2706 |
| 10 |  | A9\_1 | 0.7143 | 0.0008 | 0.3219 | 0.0005 | 1.6218 | 14.7310 |
| 11 |  | A9\_2 | 0.7217 | 0.0004 | 0.3383 | 0.0000 | 2.2507 | 14.6314 |
| 12 |  | A9\_3 | 0.7043 | 0.0014 | 0.3357 | 0.0001 | 1.9913 | 13.9384 |
| 13 |  | A9\_4 | 0.7579 | 0.0002 | 0.3378 | 0.0000 | 1.7976 | 13.1530 |
| 14 |  | A9\_6 | 0.7008 | 0.0017 | 0.3574 | 0.0002 | 1.8716 | 12.1570 |
| 15 |  | A101 | 0.6948 | 0.0023 | 0.3332 | 0.0001 | 3.6623 | 17.6548 |
| 16 |  | A102 | 0.7260 | 0.0003 | 0.3305 | 0.0002 | 2.4996 | 17.5134 |
| 17 |  | A103 | 0.7515 | 0.0001 | 0.3285 | 0.0003 | 2.4729 | 16.3788 |
| 18 |  | A104 | 0.7578 | 0.0002 | 0.3089 | 0.0013 | 2.7982 | 16.0056 |
| 19 |  | A105 | 0.7129 | 0.0009 | 0.3230 | 0.0005 | 2.5071 | 16.3191 |
| 20 | 214 | A041 | 0.7580 | 0.0002 | 0.3570 | 0.0002 | 4.2822 | 19.1180 |
| 21 |  | A042 | 0.7462 | 0.0000 | 0.3445 | 0.0000 | 2.4304 | 15.8981 |
| 22 |  | A043 | 0.7449 | 0.0000 | 0.3470 | 0.0000 | 2.6840 | 14.6777 |
| 23 |  | A044 | 0.7300 | 0.0002 | 0.3486 | 0.0000 | 1.9913 | 17.2798 |
| 24 |  | A51 | 0.7822 | 0.0016 | 0.3624 | 0.0003 | 2.6381 | 14.8375 |
| 25 |  | A52 | 0.7515 | 0.0001 | 0.3565 | 0.0001 | 2.7627 | 16.2762 |
| 26 |  | A53 | 0.7515 | 0.0001 | 0.3818 | 0.0014 | 2.5722 | 16.2867 |
| 27 |  | A6\_1 | 0.7211 | 0.0004 | 0.3476 | 0.0000 | 1.3857 | 11.0105 |
| 28 |  | A6\_3 | 0.7785 | 0.0013 | 0.3361 | 0.0001 | 2.0295 | 11.9825 |
| 29 |  | A6\_4 | 0.7260 | 0.0003 | 0.3093 | 0.0012 | 1.6878 | 13.3952 |
| 30 |  | A7\_1 | 0.7892 | 0.0022 | 0.3742 | 0.0009 | 1.8318 | 12.7752 |
| 31 | 88 | A040 | 0.6979 | 0.0020 | 0.3413 | 0.0000 | 2.1979 | 10.5792 |
| 32 |  | A041 | 0.6977 | 0.0020 | 0.3531 | 0.0001 | 2.1785 | 12.9496 |
| 33 |  | A042 | 0.7203 | 0.0005 | 0.3574 | 0.0002 | 2.4562 | 11.5614 |
| 34 |  | A043 | 0.7229 | 0.0004 | 0.3629 | 0.0003 | 2.6554 | 14.5315 |
| 35 |  | A044 | 0.7212 | 0.0004 | 0.4137 | 0.0048 | 1.5506 | 14.1101 |
| 36 |  | A050 | 0.6856 | 0.0032 | 0.3425 | 0.0000 | 1.8420 | 11.0007 |
| 37 |  | A0501 | 0.7805 | 0.0015 | 0.3498 | 0.0000 | 2.3716 | 12.5819 |
| 38 |  | A051 | 0.7622 | 0.0004 | 0.4180 | 0.0054 | 1.3488 | 13.4303 |
| 39 |  | D040 | 0.7409 | 0.0000 | 0.3387 | 0.0000 | 2.8804 | 15.8376 |
| 40 |  | D041 | 0.7877 | 0.0021 | 0.3598 | 0.0002 | 2.3238 | 15.7640 |
| 41 |  | D042 | 0.7160 | 0.0007 | 0.3237 | 0.0004 | 2.3629 | 16.1426 |
| 42 |  | D043 | 0.7551 | 0.0002 | 0.3455 | 0.0000 | 1.8452 | 16.1951 |
| 43 |  | D044 | 0.7428 | 0.0000 | 0.3553 | 0.0001 | 2.8677 | 15.3444 |
| 44 |  | D045 | 0.7844 | 0.0018 | 0.3294 | 0.0002 | 1.8078 | 14.8411 |
| 45 |  | D051 | 0.7549 | 0.0002 | 0.3274 | 0.0003 | 3.4400 | 22.0735 |
| 46 |  | D052 | 0.7177 | 0.0006 | 0.3096 | 0.0012 | 3.3929 | 22.0558 |
|  |  | Sum | 0.7397 |  | 0.3433 |  | 2.27 | 14.78 |
|  |  | Error |  | 0.0042 |  | 0.0016 |  |  |
|  |  | c(Ni) | 0.2577 |  | 0.6556 |  |  |  |