

# Supporting Information

## Insight into the Effect of Promoter Mn on Ethanol Formation from Syngas on Mn-Promoted MnCu(211) Surface: A Comparison with Cu(211) Surface

Riguang Zhang, Guiru Wang, Baojun Wang\*, Lixia Ling

*(Key Laboratory of Coal Science and Technology of Ministry of Education and Shanxi Province, Taiyuan University of Technology, Taiyuan 030024, Shanxi, People's Republic of China)*

**Table S1** The only imaginary frequency corresponding to the transition state involved in ethanol synthesis from syngas on MnCu(211) surface.

| Transition state | Imaginary frequency/cm <sup>-1</sup> |
|------------------|--------------------------------------|
| TS1              | 465.6i                               |
| TS2              | 1225.5i                              |
| TS3              | 898.9i                               |
| TS4              | 381.1i                               |
| TS5              | 381.3i                               |
| TS6              | 1044.6i                              |
| TS7              | 392.0i                               |
| TS8              | 655.1i                               |
| TS9              | 334.3i                               |

\* Corresponding author at: No. 79 Yingze West Street, Taiyuan 030024, China. Tel.: +86 351 6018239; Fax: +86 351 6041237  
E-mail address: [wangbaojun@tyut.edu.cn](mailto:wangbaojun@tyut.edu.cn); [quantumtyut@126.com](mailto:quantumtyut@126.com) (Baojun Wang)

|      |         |
|------|---------|
| TS10 | 108.1i  |
| TS11 | 205.6i  |
| TS12 | 1364.2i |
| TS13 | 356.0i  |
| TS14 | 1039.2i |
| TS15 | 560.9i  |
| TS16 | 1362.6i |
| TS17 | 1140.7i |
| TS18 | 801.0i  |
| TS19 | 584.8i  |
| TS20 | 394.4i  |
| TS21 | 179.9i  |
| TS22 | 377.4i  |
| TS23 | 1276.6i |
| TS24 | 450.1i  |
| TS25 | 1128.2i |

---

**Table S2** The coordinates and energies of all the optimized structures involved in ethanol synthesis from syngas on MnCu(211) surface.

| Species | Position of atom in Cartesian coordinates/Å |             |             |
|---------|---------------------------------------------|-------------|-------------|
| C       | Cu                                          | 0.000000000 | 0.000000000 |
|         | Cu                                          | 0.333929986 | 0.000050000 |
|         | Cu                                          | 0.172549993 | 0.000640000 |
|         | Cu                                          | 0.009970000 | 0.000360000 |
|         | Cu                                          | 0.333330005 | 0.166669995 |
|         | Cu                                          | 0.005900000 | 0.167080000 |
|         | Cu                                          | 0.166669995 | 0.166669995 |
|         | Cu                                          | 0.337960005 | 0.167710006 |
|         | Cu                                          | 0.000000000 | 0.333330005 |
|         | Cu                                          | 0.334149987 | 0.333519995 |
|         | Cu                                          | 0.173109993 | 0.333759993 |
|         | Cu                                          | 0.007980000 | 0.334259987 |
|         | Cu                                          | 0.333330005 | 0.500000000 |
|         | Cu                                          | 0.005410000 | 0.500249982 |
|         | Cu                                          | 0.166669995 | 0.500000000 |
|         | Cu                                          | 0.336820006 | 0.499689996 |
|         | Cu                                          | 0.000000000 | 0.666670024 |
|         | Cu                                          | 0.333819985 | 0.666299999 |
|         | Cu                                          | 0.172800004 | 0.666570008 |
|         | Cu                                          | 0.007960000 | 0.666779995 |
|         | Cu                                          | 0.333330005 | 0.833339989 |
|         | Cu                                          | 0.005920000 | 0.833350003 |
|         | Cu                                          | 0.166669995 | 0.833339989 |
|         | Cu                                          | 0.335689992 | 0.833599985 |
|         | Cu                                          | 0.500000000 | 0.000000000 |
|         | Cu                                          | 0.832899988 | 0.000230000 |
|         | Cu                                          | 0.673600018 | 0.001440000 |
|         | Cu                                          | 0.501879990 | 0.996569991 |
|         | Cu                                          | 0.833329976 | 0.166669995 |
|         | Cu                                          | 0.505710006 | 0.166189998 |
|         | Cu                                          | 0.666670024 | 0.166669995 |
|         | Cu                                          | 0.843750000 | 0.165409997 |
|         | Cu                                          | 0.500000000 | 0.333330005 |
|         | Cu                                          | 0.834410012 | 0.333119988 |
|         | Cu                                          | 0.678810000 | 0.329200000 |
|         | Cu                                          | 0.833329976 | 0.500000000 |
|         | Cu                                          | 0.507770002 | 0.498329997 |
|         | Cu                                          | 0.666670024 | 0.500000000 |
|         | Cu                                          | 0.842410028 | 0.500649989 |

|                                 |                |             |             |
|---------------------------------|----------------|-------------|-------------|
|                                 | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|                                 | Cu 0.833509982 | 0.667200029 | 0.147679999 |
|                                 | Cu 0.677200019 | 0.672559977 | 0.256060004 |
|                                 | Cu 0.498569995 | 0.675750017 | 0.350829989 |
|                                 | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|                                 | Cu 0.505400002 | 0.832949996 | 0.197620004 |
|                                 | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|                                 | Cu 0.843720019 | 0.836269975 | 0.299600005 |
|                                 | Mn 0.504729986 | 0.326350003 | 0.363530010 |
|                                 | C 0.598980010  | 0.498160005 | 0.321280003 |
| <b>H</b><br><b>(bridge-T-1)</b> | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|                                 | Cu 0.333609998 | 0.000280000 | 0.147860005 |
|                                 | Cu 0.171489999 | 0.001460000 | 0.251100004 |
|                                 | Cu 0.004940000 | 0.999589980 | 0.344669998 |
|                                 | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|                                 | Cu 0.005170000 | 0.167129993 | 0.198699996 |
|                                 | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|                                 | Cu 0.339020014 | 0.166730002 | 0.300139993 |
|                                 | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|                                 | Cu 0.333530009 | 0.334019989 | 0.150169998 |
|                                 | Cu 0.173109993 | 0.334650010 | 0.252499998 |
|                                 | Cu 0.005560000 | 0.333020002 | 0.344669998 |
|                                 | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|                                 | Cu 0.005340000 | 0.500270009 | 0.198829994 |
|                                 | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|                                 | Cu 0.337819993 | 0.500360012 | 0.304569989 |
|                                 | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|                                 | Cu 0.333460003 | 0.665740013 | 0.149969995 |
|                                 | Cu 0.172020003 | 0.667270005 | 0.251509994 |
|                                 | Cu 0.005180000 | 0.666339993 | 0.344660014 |
|                                 | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|                                 | Cu 0.004490000 | 0.833389997 | 0.198489994 |
|                                 | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|                                 | Cu 0.335889995 | 0.837559998 | 0.298619986 |
|                                 | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|                                 | Cu 0.832610011 | 0.000070000 | 0.149079993 |
|                                 | Cu 0.672299981 | 0.000140000 | 0.253630012 |
|                                 | Cu 0.503840029 | 0.996749997 | 0.343750000 |
|                                 | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|                                 | Cu 0.505940020 | 0.167290002 | 0.198559999 |
|                                 | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|                                 | Cu 0.838750005 | 0.166280001 | 0.300989985 |
|                                 | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|                                 | Cu 0.835060000 | 0.333420008 | 0.147139996 |

|                                |                |             |             |
|--------------------------------|----------------|-------------|-------------|
|                                | Cu 0.675970018 | 0.332529992 | 0.248649999 |
|                                | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|                                | Cu 0.506320000 | 0.498670012 | 0.197840005 |
|                                | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|                                | Cu 0.838469982 | 0.499500006 | 0.300559998 |
|                                | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|                                | Cu 0.832149982 | 0.666570008 | 0.149130002 |
|                                | Cu 0.670899987 | 0.665139973 | 0.254790008 |
|                                | Cu 0.502009988 | 0.673229992 | 0.347020000 |
|                                | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|                                | Cu 0.505810022 | 0.831439972 | 0.198139995 |
|                                | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|                                | Cu 0.838140011 | 0.832690001 | 0.300790012 |
|                                | Mn 0.515250027 | 0.333119988 | 0.355549991 |
|                                | H 0.426739991  | 0.517359972 | 0.396990001 |
| <b>H</b><br><b>(bridge-SE)</b> | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|                                | Cu 0.334199995 | 0.000420000 | 0.147900000 |
|                                | Cu 0.173209995 | 0.000300000 | 0.251049995 |
|                                | Cu 0.005560000 | 0.999939978 | 0.344049990 |
|                                | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|                                | Cu 0.005710000 | 0.166820005 | 0.198579997 |
|                                | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|                                | Cu 0.340189993 | 0.168489993 | 0.300220013 |
|                                | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|                                | Cu 0.333629996 | 0.332920015 | 0.148770005 |
|                                | Cu 0.173109993 | 0.333440006 | 0.252370000 |
|                                | Cu 0.005460000 | 0.333490014 | 0.344509989 |
|                                | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|                                | Cu 0.005810000 | 0.500090003 | 0.198689997 |
|                                | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|                                | Cu 0.339109987 | 0.500159979 | 0.298319995 |
|                                | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|                                | Cu 0.333389997 | 0.666719973 | 0.148350000 |
|                                | Cu 0.172350004 | 0.667479992 | 0.251870006 |
|                                | Cu 0.005210000 | 0.666490018 | 0.344619989 |
|                                | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|                                | Cu 0.005200000 | 0.833429992 | 0.198469996 |
|                                | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|                                | Cu 0.338880002 | 0.833239973 | 0.298359990 |
|                                | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|                                | Cu 0.832480013 | 0.000200000 | 0.148980007 |
|                                | Cu 0.672209978 | 0.000780000 | 0.254579991 |
|                                | Cu 0.503289998 | 0.997280002 | 0.344170004 |
|                                | Cu 0.833329976 | 0.166669995 | 0.000000000 |

|   |                |             |             |
|---|----------------|-------------|-------------|
|   | Cu 0.506179988 | 0.168259993 | 0.199709997 |
|   | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|   | Cu 0.838949978 | 0.166749999 | 0.300550014 |
|   | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|   | Cu 0.835219979 | 0.333200008 | 0.147100002 |
|   | Cu 0.675939977 | 0.332690001 | 0.248310000 |
|   | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|   | Cu 0.506030023 | 0.499590009 | 0.198970005 |
|   | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|   | Cu 0.838989973 | 0.499900013 | 0.300029993 |
|   | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|   | Cu 0.833369970 | 0.666710019 | 0.148410007 |
|   | Cu 0.673169971 | 0.666499972 | 0.251859993 |
|   | Cu 0.506569982 | 0.671790004 | 0.349970013 |
|   | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|   | Cu 0.505990028 | 0.830649972 | 0.199310005 |
|   | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|   | Cu 0.838779986 | 0.833360016 | 0.300319999 |
|   | Mn 0.515600026 | 0.335509986 | 0.358759999 |
|   | H 0.531960011  | 0.525409997 | 0.425529987 |
| O | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|   | Cu 0.333790004 | 0.000010000 | 0.147070006 |
|   | Cu 0.171499997 | 0.999800026 | 0.250690013 |
|   | Cu 0.004940000 | 0.000550000 | 0.344300002 |
|   | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|   | Cu 0.004830000 | 0.166669995 | 0.198269993 |
|   | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|   | Cu 0.340090007 | 0.163090006 | 0.297459990 |
|   | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|   | Cu 0.333169997 | 0.334870011 | 0.150549993 |
|   | Cu 0.172110006 | 0.333189994 | 0.251700014 |
|   | Cu 0.005070000 | 0.333829999 | 0.344309986 |
|   | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|   | Cu 0.004690000 | 0.500039995 | 0.198440000 |
|   | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|   | Cu 0.334190011 | 0.497979999 | 0.309159994 |
|   | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|   | Cu 0.333070010 | 0.664439976 | 0.150240004 |
|   | Cu 0.171590000 | 0.665059984 | 0.251540005 |
|   | Cu 0.004850000 | 0.667060018 | 0.344410002 |
|   | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|   | Cu 0.004730000 | 0.833209991 | 0.198109999 |
|   | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|   | Cu 0.337000012 | 0.835080028 | 0.296420008 |

|    |                |             |             |
|----|----------------|-------------|-------------|
|    | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|    | Cu 0.832669973 | 0.000120000 | 0.148829997 |
|    | Cu 0.672940016 | 0.001960000 | 0.253549993 |
|    | Cu 0.504869998 | 0.994189978 | 0.341439992 |
|    | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|    | Cu 0.506299973 | 0.169100001 | 0.198630005 |
|    | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|    | Cu 0.838490009 | 0.167549998 | 0.301109999 |
|    | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|    | Cu 0.834500015 | 0.333350003 | 0.147210002 |
|    | Cu 0.675180018 | 0.334479988 | 0.248769999 |
|    | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|    | Cu 0.504999995 | 0.499060005 | 0.199780002 |
|    | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|    | Cu 0.838259995 | 0.500689983 | 0.300529987 |
|    | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|    | Cu 0.832930028 | 0.666819990 | 0.148220003 |
|    | Cu 0.672599971 | 0.667509973 | 0.251569986 |
|    | Cu 0.507600009 | 0.677929997 | 0.347629994 |
|    | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|    | Cu 0.506399989 | 0.831369996 | 0.197170004 |
|    | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|    | Cu 0.838689983 | 0.833949983 | 0.300680012 |
|    | Mn 0.519349992 | 0.323049992 | 0.361950010 |
|    | O 0.435849994  | 0.496439993 | 0.411500007 |
| OH | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|    | Cu 0.334179997 | 0.000490000 | 0.148069993 |
|    | Cu 0.173730001 | 0.000520000 | 0.250910014 |
|    | Cu 0.005640000 | 0.000030000 | 0.344319999 |
|    | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|    | Cu 0.006080000 | 0.166970000 | 0.198469996 |
|    | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|    | Cu 0.340620011 | 0.170059994 | 0.300029993 |
|    | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|    | Cu 0.334010005 | 0.333079994 | 0.148550004 |
|    | Cu 0.173429996 | 0.333620012 | 0.252440006 |
|    | Cu 0.005210000 | 0.333649993 | 0.344330013 |
|    | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|    | Cu 0.006090000 | 0.500180006 | 0.198440000 |
|    | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|    | Cu 0.339679986 | 0.500590026 | 0.297679991 |
|    | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|    | Cu 0.333770007 | 0.666790009 | 0.148179993 |
|    | Cu 0.172749996 | 0.668009996 | 0.251839995 |

|    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|    | Cu 0.005000000 0.666459978 0.344540000<br>Cu 0.333330005 0.833339989 0.000000000<br>Cu 0.005710000 0.833689988 0.198320001<br>Cu 0.166669995 0.833339989 0.097309999<br>Cu 0.339179993 0.832920015 0.297950000<br>Cu 0.500000000 0.000000000 0.048650000<br>Cu 0.832769990 0.000440000 0.148969993<br>Cu 0.672689974 0.001150000 0.253939986<br>Cu 0.503170013 0.999319971 0.343829989<br>Cu 0.833329976 0.166669995 0.000000000<br>Cu 0.505840003 0.168819994 0.199790001<br>Cu 0.666670024 0.166669995 0.097309999<br>Cu 0.839030027 0.166940004 0.300630003<br>Cu 0.500000000 0.333330005 0.048650000<br>Cu 0.835210025 0.333389997 0.147170007<br>Cu 0.676370025 0.332850009 0.247920007<br>Cu 0.833329976 0.500000000 0.000000000<br>Cu 0.506420016 0.499350011 0.200650007<br>Cu 0.666670024 0.500000000 0.097309999<br>Cu 0.839219987 0.500050008 0.299970001<br>Cu 0.500000000 0.666670024 0.048650000<br>Cu 0.833850026 0.666930020 0.148029998<br>Cu 0.674229980 0.666570008 0.250589997<br>Cu 0.509239972 0.677890003 0.351779997<br>Cu 0.833329976 0.833339989 0.000000000<br>Cu 0.505649984 0.829800010 0.199650005<br>Cu 0.666670024 0.833339989 0.097309999<br>Cu 0.838869989 0.833440006 0.300390005<br>Mn 0.518930018 0.330119997 0.361919999<br>O 0.541719973 0.511950016 0.450890005<br>H 0.614950001 0.528230011 0.470530003 |
| CO | Cu 0.000000000 0.000000000 0.048650000<br>Cu 0.333819985 0.000360000 0.147919998<br>Cu 0.171619996 0.999700010 0.250779986<br>Cu 0.004380000 0.999750018 0.344379991<br>Cu 0.333330005 0.166669995 0.000000000<br>Cu 0.004880000 0.166580006 0.198630005<br>Cu 0.166669995 0.166669995 0.097309999<br>Cu 0.338950008 0.165240005 0.299879998<br>Cu 0.000000000 0.333330005 0.048650000<br>Cu 0.333669990 0.334120005 0.149990007<br>Cu 0.172460005 0.333149999 0.251729995<br>Cu 0.005060000 0.333139986 0.344500005<br>Cu 0.333330005 0.500000000 0.000000000                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |



|    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|    | Cu 0.005040000 0.499879986 0.198840007<br>Cu 0.166669995 0.500000000 0.097309999<br>Cu 0.336919993 0.498219997 0.305770010<br>Cu 0.000000000 0.666670024 0.048650000<br>Cu 0.333240002 0.665499985 0.149869993<br>Cu 0.171979994 0.666130006 0.251639992<br>Cu 0.004790000 0.666589975 0.344500005<br>Cu 0.333330005 0.833339989 0.000000000<br>Cu 0.004390000 0.833019972 0.198500007<br>Cu 0.166669995 0.833339989 0.097309999<br>Cu 0.336970001 0.834860027 0.298440009<br>Cu 0.500000000 0.000000000 0.048650000<br>Cu 0.832830012 0.000120000 0.148839995<br>Cu 0.672379971 0.000560000 0.252700001<br>Cu 0.504059970 0.997609973 0.344379991<br>Cu 0.833329976 0.166669995 0.000000000<br>Cu 0.506079972 0.168459997 0.198990002<br>Cu 0.666670024 0.166669995 0.097309999<br>Cu 0.838220000 0.166769996 0.300989985<br>Cu 0.500000000 0.333330005 0.048650000<br>Cu 0.834169984 0.333209991 0.147740006<br>Cu 0.674399972 0.333400011 0.249630004<br>Cu 0.833329976 0.500000000 0.000000000<br>Cu 0.505630016 0.500360012 0.197819993<br>Cu 0.666670024 0.500000000 0.097309999<br>Cu 0.838100016 0.499720007 0.300650001<br>Cu 0.500000000 0.666670024 0.048650000<br>Cu 0.832690001 0.666440010 0.148709998<br>Cu 0.671739995 0.665440023 0.252929986<br>Cu 0.505020022 0.672010005 0.346940011<br>Cu 0.833329976 0.833339989 0.000000000<br>Cu 0.505559981 0.833029985 0.198039994<br>Cu 0.666670024 0.833339989 0.097309999<br>Cu 0.837939978 0.833010018 0.300830007<br>Mn 0.512480021 0.335390002 0.355890006<br>C 0.427740008 0.493869990 0.432810009<br>O 0.390789986 0.529969990 0.502659976 |
| CH | Cu 0.000000000 0.000000000 0.048650000<br>Cu 0.333290011 0.999890029 0.148379996<br>Cu 0.172800004 0.998939991 0.251280010<br>Cu 0.007780000 0.000250000 0.344579995<br>Cu 0.333330005 0.166669995 0.000000000<br>Cu 0.005930000 0.166820005 0.198180005<br>Cu 0.166669995 0.166669995 0.097309999                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |

|  |                |             |             |
|--|----------------|-------------|-------------|
|  | Cu 0.338759989 | 0.166779995 | 0.300729990 |
|  | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|  | Cu 0.332870007 | 0.332419991 | 0.149049997 |
|  | Cu 0.173040003 | 0.333339989 | 0.252370000 |
|  | Cu 0.006210000 | 0.334509999 | 0.344520003 |
|  | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|  | Cu 0.004340000 | 0.499949992 | 0.199169993 |
|  | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|  | Cu 0.339040011 | 0.498769999 | 0.301569998 |
|  | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|  | Cu 0.332679987 | 0.666769981 | 0.148650005 |
|  | Cu 0.172629997 | 0.665690005 | 0.251989990 |
|  | Cu 0.006030000 | 0.666450024 | 0.344619989 |
|  | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|  | Cu 0.005400000 | 0.833050013 | 0.198180005 |
|  | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|  | Cu 0.339150012 | 0.829509974 | 0.299980015 |
|  | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|  | Cu 0.833519995 | 0.000160000 | 0.148359999 |
|  | Cu 0.672420025 | 0.001590000 | 0.251760006 |
|  | Cu 0.502550006 | 0.994560003 | 0.343510002 |
|  | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|  | Cu 0.505150020 | 0.167769998 | 0.199059993 |
|  | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|  | Cu 0.841570020 | 0.165350005 | 0.299400002 |
|  | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|  | Cu 0.834140003 | 0.333579987 | 0.147469997 |
|  | Cu 0.675880015 | 0.334459990 | 0.251800001 |
|  | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|  | Cu 0.502380013 | 0.499049991 | 0.195160002 |
|  | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|  | Cu 0.838729978 | 0.500880003 | 0.302390009 |
|  | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|  | Cu 0.833339989 | 0.666639984 | 0.147919998 |
|  | Cu 0.674070001 | 0.667840004 | 0.252640009 |
|  | Cu 0.508889973 | 0.667800009 | 0.345800012 |
|  | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|  | Cu 0.504710019 | 0.833109975 | 0.196909994 |
|  | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|  | Cu 0.841139972 | 0.836210012 | 0.299409986 |
|  | Mn 0.513390005 | 0.332239985 | 0.358229995 |
|  | C 0.635589957  | 0.501800001 | 0.353850007 |
|  | H 0.680960000  | 0.515850008 | 0.415609986 |

|                 |                |             |             |
|-----------------|----------------|-------------|-------------|
| CH <sub>2</sub> | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|                 | Cu 0.334089994 | 0.000710000 | 0.148080006 |
|                 | Cu 0.172600001 | 0.000320000 | 0.251179993 |
|                 | Cu 0.004940000 | 0.000130000 | 0.343890011 |
|                 | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|                 | Cu 0.005390000 | 0.166810006 | 0.198300004 |
|                 | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|                 | Cu 0.340420008 | 0.167940006 | 0.300249994 |
|                 | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|                 | Cu 0.334019989 | 0.332549989 | 0.148650005 |
|                 | Cu 0.173150003 | 0.333119988 | 0.252200007 |
|                 | Cu 0.005210000 | 0.333519995 | 0.343989998 |
|                 | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|                 | Cu 0.005890000 | 0.500039995 | 0.198330000 |
|                 | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|                 | Cu 0.339300007 | 0.499599993 | 0.297500014 |
|                 | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|                 | Cu 0.333889991 | 0.666920006 | 0.148420006 |
|                 | Cu 0.172549993 | 0.667129993 | 0.251679987 |
|                 | Cu 0.005070000 | 0.666700006 | 0.344150007 |
|                 | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|                 | Cu 0.005280000 | 0.833410025 | 0.198239997 |
|                 | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|                 | Cu 0.338629991 | 0.834429979 | 0.297789991 |
|                 | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|                 | Cu 0.832620025 | 0.000170000 | 0.148839995 |
|                 | Cu 0.671989977 | 0.000800000 | 0.253719985 |
|                 | Cu 0.504069984 | 0.997200012 | 0.345450014 |
|                 | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|                 | Cu 0.505710006 | 0.167750001 | 0.199919999 |
|                 | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|                 | Cu 0.838329971 | 0.167030007 | 0.300440013 |
|                 | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|                 | Cu 0.834469974 | 0.333339989 | 0.147450000 |
|                 | Cu 0.674700022 | 0.333050013 | 0.248950005 |
|                 | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|                 | Cu 0.505959988 | 0.498989999 | 0.199910000 |
|                 | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|                 | Cu 0.838769972 | 0.499989986 | 0.299589992 |
|                 | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|                 | Cu 0.833809972 | 0.666649997 | 0.147990003 |
|                 | Cu 0.673330009 | 0.666760027 | 0.250569999 |
|                 | Cu 0.506699979 | 0.674070001 | 0.351579994 |
|                 | Cu 0.833329976 | 0.833339989 | 0.000000000 |

|                 |                |             |             |
|-----------------|----------------|-------------|-------------|
|                 | Cu 0.505779982 | 0.831179976 | 0.198919997 |
|                 | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|                 | Cu 0.838540018 | 0.833440006 | 0.300020009 |
|                 | Mn 0.515330017 | 0.332410008 | 0.362819999 |
|                 | C 0.521130025  | 0.516799986 | 0.452840000 |
|                 | H 0.598779976  | 0.538330019 | 0.484679997 |
|                 | H 0.454109997  | 0.528479993 | 0.499049991 |
| CH <sub>3</sub> | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|                 | Cu 0.334280014 | 0.000330000 | 0.147939995 |
|                 | Cu 0.173470005 | 0.000180000 | 0.251069993 |
|                 | Cu 0.005800000 | 0.999970019 | 0.344090015 |
|                 | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|                 | Cu 0.005970000 | 0.166789994 | 0.198589996 |
|                 | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|                 | Cu 0.340270013 | 0.168799996 | 0.300170004 |
|                 | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|                 | Cu 0.333559990 | 0.332789987 | 0.148499995 |
|                 | Cu 0.173140004 | 0.333409995 | 0.252810001 |
|                 | Cu 0.005400000 | 0.333499998 | 0.344630003 |
|                 | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|                 | Cu 0.006080000 | 0.500090003 | 0.198630005 |
|                 | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|                 | Cu 0.339329988 | 0.500199974 | 0.297520012 |
|                 | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|                 | Cu 0.333380014 | 0.666960001 | 0.148059994 |
|                 | Cu 0.172470003 | 0.667460024 | 0.252200007 |
|                 | Cu 0.005270000 | 0.666509986 | 0.344680011 |
|                 | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|                 | Cu 0.005420000 | 0.833400011 | 0.198469996 |
|                 | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|                 | Cu 0.339179993 | 0.832719982 | 0.298280001 |
|                 | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|                 | Cu 0.832499981 | 0.000220000 | 0.149049997 |
|                 | Cu 0.672420025 | 0.000900000 | 0.254790008 |
|                 | Cu 0.503199995 | 0.997739971 | 0.343910009 |
|                 | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|                 | Cu 0.506380022 | 0.168809995 | 0.199790001 |
|                 | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|                 | Cu 0.839150012 | 0.166830003 | 0.300619990 |
|                 | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|                 | Cu 0.835370004 | 0.333149999 | 0.147009999 |
|                 | Cu 0.676209986 | 0.332910001 | 0.248119995 |
|                 | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|                 | Cu 0.506210029 | 0.499989986 | 0.199520007 |

|                 |                |             |             |
|-----------------|----------------|-------------|-------------|
|                 | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|                 | Cu 0.839259982 | 0.500000000 | 0.299950004 |
|                 | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|                 | Cu 0.833379984 | 0.666750014 | 0.148450002 |
|                 | Cu 0.673489988 | 0.666559994 | 0.251890004 |
|                 | Cu 0.506550014 | 0.670029998 | 0.351269990 |
|                 | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|                 | Cu 0.506299973 | 0.829819977 | 0.200010002 |
|                 | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|                 | Cu 0.838940024 | 0.833369970 | 0.300430000 |
|                 | Mn 0.515009999 | 0.337240010 | 0.358260006 |
|                 | C 0.542159975  | 0.515500009 | 0.465860009 |
|                 | H 0.618330002  | 0.449180007 | 0.479999989 |
|                 | H 0.555920005  | 0.652840018 | 0.485000014 |
|                 | H 0.479209989  | 0.467260003 | 0.510219991 |
| CH <sub>4</sub> | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|                 | Cu 0.333609998 | 0.000230000 | 0.149350002 |
|                 | Cu 0.172470003 | 0.000150000 | 0.252519995 |
|                 | Cu 0.005370000 | 0.000100000 | 0.345560014 |
|                 | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|                 | Cu 0.005420000 | 0.166559994 | 0.199379995 |
|                 | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|                 | Cu 0.340009987 | 0.167579994 | 0.302010000 |
|                 | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|                 | Cu 0.333710015 | 0.333229989 | 0.149590001 |
|                 | Cu 0.173360005 | 0.333039999 | 0.253100008 |
|                 | Cu 0.005820000 | 0.333440006 | 0.345569998 |
|                 | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|                 | Cu 0.005450000 | 0.500039995 | 0.199379995 |
|                 | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|                 | Cu 0.339749992 | 0.498369992 | 0.301950008 |
|                 | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|                 | Cu 0.333559990 | 0.666339993 | 0.149320006 |
|                 | Cu 0.172440007 | 0.666050017 | 0.252510011 |
|                 | Cu 0.005410000 | 0.666859984 | 0.345560014 |
|                 | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|                 | Cu 0.004800000 | 0.833329976 | 0.199239999 |
|                 | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|                 | Cu 0.336109996 | 0.832840025 | 0.300669998 |
|                 | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|                 | Cu 0.832490027 | 0.000180000 | 0.150089994 |
|                 | Cu 0.671729982 | 0.001450000 | 0.255879998 |
|                 | Cu 0.502550006 | 0.994140029 | 0.345860004 |
|                 | Cu 0.833329976 | 0.166669995 | 0.000000000 |

|     |                |             |             |
|-----|----------------|-------------|-------------|
|     | Cu 0.505739987 | 0.167630002 | 0.199780002 |
|     | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|     | Cu 0.838609993 | 0.167229995 | 0.301840007 |
|     | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|     | Cu 0.835860014 | 0.333380014 | 0.147440001 |
|     | Cu 0.676699996 | 0.333840013 | 0.248410001 |
|     | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|     | Cu 0.505670011 | 0.499020010 | 0.199579999 |
|     | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|     | Cu 0.838689983 | 0.499890000 | 0.301789999 |
|     | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|     | Cu 0.832579970 | 0.666599989 | 0.150000006 |
|     | Cu 0.671880007 | 0.665939987 | 0.255589992 |
|     | Cu 0.502669990 | 0.670289993 | 0.345950007 |
|     | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|     | Cu 0.505469978 | 0.833239973 | 0.198359996 |
|     | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|     | Cu 0.838110030 | 0.833549976 | 0.301899999 |
|     | Mn 0.518280029 | 0.333499998 | 0.358639985 |
|     | C 0.635890007  | 0.332399994 | 0.545120001 |
|     | H 0.605620027  | 0.214910001 | 0.511990011 |
|     | H 0.613810003  | 0.451009989 | 0.508759975 |
|     | H 0.602039993  | 0.338869989 | 0.611679971 |
|     | H 0.723119974  | 0.324539989 | 0.547930002 |
| COH | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|     | Cu 0.333180010 | 0.001990000 | 0.149690002 |
|     | Cu 0.170959994 | 0.999530017 | 0.251729995 |
|     | Cu 0.004010000 | 0.000410000 | 0.344669998 |
|     | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|     | Cu 0.004700000 | 0.166429996 | 0.198660001 |
|     | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|     | Cu 0.336210012 | 0.165279999 | 0.303570002 |
|     | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|     | Cu 0.333689988 | 0.333559990 | 0.148800001 |
|     | Cu 0.171959996 | 0.333149999 | 0.251210004 |
|     | Cu 0.004460000 | 0.333400011 | 0.344069988 |
|     | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|     | Cu 0.004740000 | 0.499980003 | 0.198650002 |
|     | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|     | Cu 0.336809993 | 0.500159979 | 0.305729985 |
|     | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|     | Cu 0.333260000 | 0.664929986 | 0.149700001 |
|     | Cu 0.171379998 | 0.665809989 | 0.251610011 |
|     | Cu 0.004090000 | 0.666719973 | 0.344469994 |

|            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|            | Cu 0.333330005 0.833339989 0.000000000<br>Cu 0.004200000 0.833180010 0.198220000<br>Cu 0.166669995 0.833339989 0.097309999<br>Cu 0.336100012 0.832759976 0.299299985<br>Cu 0.500000000 0.000000000 0.048650000<br>Cu 0.832560003 0.000110000 0.148670003<br>Cu 0.671589971 0.001070000 0.253100008<br>Cu 0.503520012 0.997330010 0.344190001<br>Cu 0.833329976 0.166669995 0.000000000<br>Cu 0.505750000 0.168180004 0.198339999<br>Cu 0.666670024 0.166669995 0.097309999<br>Cu 0.837539971 0.166769996 0.300920010<br>Cu 0.500000000 0.333330005 0.048650000<br>Cu 0.834649980 0.333299994 0.147269994<br>Cu 0.674979985 0.333370000 0.248620003<br>Cu 0.833329976 0.500000000 0.000000000<br>Cu 0.505439997 0.499229997 0.198609993<br>Cu 0.666670024 0.500000000 0.097309999<br>Cu 0.837580025 0.500069976 0.300920010<br>Cu 0.500000000 0.666670024 0.048650000<br>Cu 0.832700014 0.666520000 0.148570001<br>Cu 0.671809971 0.665669978 0.252739996<br>Cu 0.504220009 0.671739995 0.344220012<br>Cu 0.833329976 0.833339989 0.000000000<br>Cu 0.504710019 0.833840013 0.197160006<br>Cu 0.666670024 0.833339989 0.097309999<br>Cu 0.837849975 0.833459973 0.300660014<br>Mn 0.516319990 0.334719986 0.358559996<br>C 0.371300012 0.329230011 0.401190013<br>O 0.323879987 0.327850014 0.480690002<br>H 0.246439993 0.320190012 0.473500013 |
| <b>CHO</b> | Cu 0.000000000 0.000000000 0.048650000<br>Cu 0.334320009 0.001050000 0.148029998<br>Cu 0.173700005 0.000330000 0.250959992<br>Cu 0.005860000 0.000320000 0.344099998<br>Cu 0.333330005 0.166669995 0.000000000<br>Cu 0.005650000 0.166909993 0.198620006<br>Cu 0.166669995 0.166669995 0.097309999<br>Cu 0.341179997 0.168740004 0.300159991<br>Cu 0.000000000 0.333330005 0.048650000<br>Cu 0.334540009 0.332830012 0.148990005<br>Cu 0.174040005 0.333490014 0.251650006<br>Cu 0.006000000 0.333600014 0.344110012<br>Cu 0.333330005 0.500000000 0.000000000                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |

|                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                        | Cu 0.005850000 0.500109971 0.198809996<br>Cu 0.166669995 0.500000000 0.097309999<br>Cu 0.339740008 0.500460029 0.298469990<br>Cu 0.000000000 0.666670024 0.048650000<br>Cu 0.334089994 0.666400015 0.148399994<br>Cu 0.173319995 0.667519987 0.251170009<br>Cu 0.006130000 0.666819990 0.344370008<br>Cu 0.333330005 0.833339989 0.000000000<br>Cu 0.005430000 0.833580017 0.198780000<br>Cu 0.166669995 0.833339989 0.097309999<br>Cu 0.339709997 0.833329976 0.298409998<br>Cu 0.500000000 0.000000000 0.048650000<br>Cu 0.833090007 0.000050000 0.148469999<br>Cu 0.673169971 0.000370000 0.252469987<br>Cu 0.505410016 0.999029994 0.343230009<br>Cu 0.833329976 0.166669995 0.000000000<br>Cu 0.506330013 0.169430003 0.200330004<br>Cu 0.666670024 0.166669995 0.097309999<br>Cu 0.839039981 0.166869998 0.300579995<br>Cu 0.500000000 0.333330005 0.048650000<br>Cu 0.834110022 0.333389997 0.147630006<br>Cu 0.674839973 0.333600014 0.249819994<br>Cu 0.833329976 0.500000000 0.000000000<br>Cu 0.506460011 0.498860002 0.199760005<br>Cu 0.666670024 0.500000000 0.097309999<br>Cu 0.839230001 0.500169992 0.300370008<br>Cu 0.500000000 0.666670024 0.048650000<br>Cu 0.833589971 0.666729987 0.148220003<br>Cu 0.673879981 0.666360021 0.251320004<br>Cu 0.511160016 0.672129989 0.349379987<br>Cu 0.833329976 0.833339989 0.000000000<br>Cu 0.505140007 0.830810010 0.199029997<br>Cu 0.666670024 0.833339989 0.097309999<br>Cu 0.838959992 0.833500028 0.300700009<br>Mn 0.515919983 0.333790004 0.363370001<br>H 0.517700016 0.677789986 0.522199988<br>C 0.518649995 0.581120014 0.467489988<br>O 0.524619997 0.424540013 0.492240012 |
| <b>CH<sub>2</sub>O</b> | Cu 0.000000000 0.000000000 0.048650000<br>Cu 0.334320009 0.000450000 0.148770005<br>Cu 0.173189998 0.000460000 0.252539992<br>Cu 0.005770000 0.000020000 0.345189989<br>Cu 0.333330005 0.166669995 0.000000000<br>Cu 0.005540000 0.166669995 0.199049994                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |



|  |                |             |             |
|--|----------------|-------------|-------------|
|  | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|  | Cu 0.340559989 | 0.168630004 | 0.301079988 |
|  | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|  | Cu 0.333810002 | 0.332760006 | 0.148859993 |
|  | Cu 0.173069999 | 0.333240002 | 0.253219992 |
|  | Cu 0.005600000 | 0.333480000 | 0.345380008 |
|  | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|  | Cu 0.005630000 | 0.500129998 | 0.199049994 |
|  | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|  | Cu 0.339370012 | 0.499650002 | 0.298409998 |
|  | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|  | Cu 0.333810002 | 0.666980028 | 0.148560002 |
|  | Cu 0.172590002 | 0.667110026 | 0.252730012 |
|  | Cu 0.005420000 | 0.666689992 | 0.345380008 |
|  | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|  | Cu 0.005240000 | 0.833519995 | 0.198949993 |
|  | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|  | Cu 0.338539988 | 0.833339989 | 0.299899995 |
|  | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|  | Cu 0.833100021 | 0.000130000 | 0.149230003 |
|  | Cu 0.672389984 | 0.000350000 | 0.253919989 |
|  | Cu 0.504459977 | 0.996969998 | 0.344700009 |
|  | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|  | Cu 0.505869985 | 0.169560000 | 0.201320007 |
|  | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|  | Cu 0.838739991 | 0.166869998 | 0.301270008 |
|  | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|  | Cu 0.834640026 | 0.333319992 | 0.148149997 |
|  | Cu 0.674660027 | 0.333070010 | 0.250039995 |
|  | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|  | Cu 0.505890012 | 0.498369992 | 0.200430006 |
|  | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|  | Cu 0.838750005 | 0.499929994 | 0.300929993 |
|  | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|  | Cu 0.833459973 | 0.666660011 | 0.148969993 |
|  | Cu 0.672659993 | 0.666369975 | 0.252819985 |
|  | Cu 0.506630003 | 0.668569982 | 0.351209998 |
|  | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|  | Cu 0.505439997 | 0.831009984 | 0.199699998 |
|  | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|  | Cu 0.838590026 | 0.833280027 | 0.301189989 |
|  | Mn 0.516579986 | 0.336919993 | 0.364870012 |
|  | C 0.535359979  | 0.554470003 | 0.476460010 |
|  | H 0.612450004  | 0.621410012 | 0.485390007 |

|                   |                                        |
|-------------------|----------------------------------------|
|                   | H 0.466600001 0.619090021 0.507889986  |
|                   | O 0.538190007 0.379579991 0.485229999  |
| CH <sub>3</sub> O | Cu 0.000000000 0.000000000 0.048650000 |
|                   | Cu 0.334329993 0.000540000 0.148010001 |
|                   | Cu 0.173270002 0.000270000 0.251040012 |
|                   | Cu 0.005640000 0.000180000 0.344209999 |
|                   | Cu 0.333330005 0.166669995 0.000000000 |
|                   | Cu 0.005870000 0.166679993 0.198500007 |
|                   | Cu 0.166669995 0.166669995 0.097309999 |
|                   | Cu 0.339910001 0.169170007 0.300069988 |
|                   | Cu 0.000000000 0.333330005 0.048650000 |
|                   | Cu 0.333640009 0.332870007 0.148139998 |
|                   | Cu 0.173170000 0.333449990 0.252290010 |
|                   | Cu 0.005430000 0.333539993 0.344419986 |
|                   | Cu 0.333330005 0.500000000 0.000000000 |
|                   | Cu 0.005870000 0.500079989 0.198540002 |
|                   | Cu 0.166669995 0.500000000 0.097309999 |
|                   | Cu 0.339639992 0.499900013 0.296559989 |
|                   | Cu 0.000000000 0.666670024 0.048650000 |
|                   | Cu .333499998 0.666769981 0.147850007  |
|                   | Cu 0.172509998 0.667050004 0.251800001 |
|                   | Cu 0.005260000 0.666750014 0.344529986 |
|                   | Cu 0.333330005 0.833339989 0.000000000 |
|                   | Cu 0.005500000 0.833580017 0.198369995 |
|                   | Cu 0.166669995 0.833339989 0.097309999 |
|                   | Cu 0.338479996 0.833069980 0.298060000 |
|                   | Cu 0.500000000 0.000000000 0.048650000 |
|                   | Cu 0.832660019 0.000200000 0.148969993 |
|                   | Cu 0.672360003 0.000990000 0.253740013 |
|                   | Cu 0.502860010 0.997569978 0.343250006 |
|                   | Cu 0.833329976 0.166669995 0.000000000 |
|                   | Cu 0.506139994 0.169019997 0.200020000 |
|                   | Cu 0.666670024 0.166669995 0.097309999 |
|                   | Cu 0.838819981 0.166979998 0.300500005 |
|                   | Cu 0.500000000 0.333330005 0.048650000 |
|                   | Cu 0.834909976 0.333160013 0.147369996 |
|                   | Cu 0.675440013 0.333130002 0.248370007 |
|                   | Cu 0.833329976 0.500000000 0.000000000 |
|                   | Cu 0.506560028 0.499269992 0.200780004 |
|                   | Cu 0.666670024 0.500000000 0.097309999 |
|                   | Cu 0.839010000 0.500069976 0.299910009 |
|                   | Cu 0.500000000 0.666670024 0.048650000 |
|                   | Cu 0.833689988 0.666800022 0.148190007 |
|                   | Cu 0.673709989 0.666779995 0.250829995 |

|      |                |             |             |
|------|----------------|-------------|-------------|
|      | Cu 0.506739974 | 0.676800013 | 0.350600004 |
|      | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|      | Cu 0.506049991 | 0.829729974 | 0.199589998 |
|      | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|      | Cu 0.838909984 | 0.833620012 | 0.300229996 |
|      | Mn 0.516610026 | 0.329930007 | 0.362459987 |
|      | C 0.467759997  | 0.529349983 | 0.532000005 |
|      | H 0.385010004  | 0.482780010 | 0.524930000 |
|      | H 0.465609998  | 0.667270005 | 0.551469982 |
|      | H 0.506850004  | 0.454380006 | 0.584730029 |
|      | O 0.527580023  | 0.510330021 | 0.452210009 |
|      |                |             |             |
| CHOH | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|      | Cu 0.334300011 | 0.000570000 | 0.148680001 |
|      | Cu 0.173050001 | 0.000890000 | 0.251769990 |
|      | Cu 0.005520000 | 0.999329984 | 0.344339997 |
|      | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|      | Cu 0.005690000 | 0.166800007 | 0.198660001 |
|      | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|      | Cu 0.340149999 | 0.168770000 | 0.301310003 |
|      | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|      | Cu 0.333739996 | 0.332470000 | 0.148729995 |
|      | Cu 0.173030004 | 0.333779991 | 0.253199995 |
|      | Cu 0.005330000 | 0.332890004 | 0.344790012 |
|      | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|      | Cu 0.005880000 | 0.500169992 | 0.198740005 |
|      | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|      | Cu 0.338829994 | 0.500079989 | 0.297010005 |
|      | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|      | Cu 0.333600014 | 0.667240024 | 0.148300007 |
|      | Cu 0.172570005 | 0.668020010 | 0.252680004 |
|      | Cu 0.005190000 | 0.665870011 | 0.344810009 |
|      | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|      | Cu 0.005250000 | 0.833329976 | 0.198559999 |
|      | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|      | Cu 0.338750005 | 0.833840013 | 0.299320012 |
|      | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|      | Cu 0.832780004 | 0.000100000 | 0.149059996 |
|      | Cu 0.672200024 | 0.000030000 | 0.254339993 |
|      | Cu 0.504310012 | 0.997839987 | 0.345600009 |
|      | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|      | Cu 0.506020010 | 0.168449998 | 0.200059995 |
|      | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|      | Cu 0.838829994 | 0.166160002 | 0.300610006 |
|      | Cu 0.500000000 | 0.333330005 | 0.048650000 |

|                         |                |             |             |
|-------------------------|----------------|-------------|-------------|
|                         | Cu 0.835039973 | 0.333319992 | 0.147410005 |
|                         | Cu 0.675509989 | 0.332309991 | 0.248940006 |
|                         | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|                         | Cu 0.506240010 | 0.499449998 | 0.198290005 |
|                         | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|                         | Cu 0.838810027 | 0.499300003 | 0.300170004 |
|                         | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|                         | Cu 0.833140016 | 0.666549981 | 0.148750007 |
|                         | Cu 0.672500014 | 0.665589988 | 0.252939999 |
|                         | Cu 0.506150007 | 0.669770002 | 0.351179987 |
|                         | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|                         | Cu 0.505770028 | 0.831179976 | 0.199719995 |
|                         | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|                         | Cu 0.838559985 | 0.832599998 | 0.300540000 |
|                         | Mn 0.514479995 | 0.337819993 | 0.359059989 |
|                         | C 0.514060020  | 0.509270012 | 0.458350003 |
|                         | H 0.589680016  | 0.529020011 | 0.494019985 |
|                         | H 0.365339994  | 0.516300023 | 0.487069994 |
|                         | O 0.433169991  | 0.529569983 | 0.518459976 |
| <b>CH<sub>2</sub>OH</b> | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|                         | Cu 0.334340006 | 0.001380000 | 0.148029998 |
|                         | Cu 0.173510000 | 0.001180000 | 0.251249999 |
|                         | Cu 0.005390000 | 0.999800026 | 0.343910009 |
|                         | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|                         | Cu 0.005710000 | 0.166889995 | 0.198459998 |
|                         | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|                         | Cu 0.341030002 | 0.170530006 | 0.300089985 |
|                         | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|                         | Cu 0.333519995 | 0.332630008 | 0.148259997 |
|                         | Cu 0.173219994 | 0.333970010 | 0.252819985 |
|                         | Cu 0.004900000 | 0.333339989 | 0.344220012 |
|                         | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|                         | Cu 0.005980000 | 0.500159979 | 0.198500007 |
|                         | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|                         | Cu 0.339560002 | 0.500580013 | 0.297410011 |
|                         | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|                         | Cu 0.333370000 | 0.666639984 | 0.147990003 |
|                         | Cu 0.172549993 | 0.667789996 | 0.252130002 |
|                         | Cu 0.004930000 | 0.666270018 | 0.344500005 |
|                         | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|                         | Cu 0.005580000 | 0.833630025 | 0.198400006 |
|                         | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|                         | Cu 0.339179993 | 0.834050000 | 0.297060013 |
|                         | Cu 0.500000000 | 0.000000000 | 0.048650000 |

|                    |                |             |             |
|--------------------|----------------|-------------|-------------|
|                    | Cu 0.832549989 | 0.000150000 | 0.148920000 |
|                    | Cu 0.672290027 | 0.999840021 | 0.254079998 |
|                    | Cu 0.503809988 | 0.999459982 | 0.343690008 |
|                    | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|                    | Cu 0.506290019 | 0.168669999 | 0.199689999 |
|                    | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|                    | Cu 0.838519990 | 0.166490003 | 0.300379992 |
|                    | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|                    | Cu 0.834940016 | 0.333209991 | 0.147049993 |
|                    | Cu 0.675549984 | 0.332280010 | 0.248260006 |
|                    | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|                    | Cu 0.505909979 | 0.499069989 | 0.199800000 |
|                    | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|                    | Cu 0.838769972 | 0.499590009 | 0.299699992 |
|                    | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|                    | Cu 0.833500028 | 0.666670024 | 0.148359999 |
|                    | Cu 0.673030019 | 0.665750027 | 0.251690000 |
|                    | Cu 0.506850004 | 0.671959996 | 0.351990014 |
|                    | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|                    | Cu 0.505840003 | 0.829970002 | 0.199159995 |
|                    | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|                    | Cu 0.838680029 | 0.832930028 | 0.300150007 |
|                    | Mn 0.517400026 | 0.337040007 | 0.359560013 |
|                    | C 0.533990026  | 0.589519978 | 0.474489987 |
|                    | H 0.618550003  | 0.605989993 | 0.490449995 |
|                    | H 0.484899998  | 0.671710014 | 0.517530024 |
|                    | H 0.435739994  | 0.394069999 | 0.511399984 |
|                    | O 0.511210024  | 0.403169990 | 0.496170014 |
| CH <sub>3</sub> OH | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|                    | Cu 0.333539993 | 0.000500000 | 0.148629993 |
|                    | Cu 0.172519997 | 0.000670000 | 0.251480013 |
|                    | Cu 0.004860000 | 0.000130000 | 0.344619989 |
|                    | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|                    | Cu 0.005970000 | 0.166730002 | 0.198559999 |
|                    | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|                    | Cu 0.340380013 | 0.168929994 | 0.301450014 |
|                    | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|                    | Cu 0.333249986 | 0.333229989 | 0.148880005 |
|                    | Cu 0.173150003 | 0.333310008 | 0.252790004 |
|                    | Cu 0.004470000 | 0.333400011 | 0.344870001 |
|                    | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|                    | Cu 0.005570000 | 0.499960005 | 0.198730007 |
|                    | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|                    | Cu 0.340449989 | 0.497819990 | 0.300810009 |

|                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|-------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                         | Cu 0.000000000 0.666670024 0.048650000<br>Cu 0.333480000 0.666170001 0.148599997<br>Cu 0.172299996 0.665849984 0.251459986<br>Cu 0.004670000 0.666540027 0.344700009<br>Cu 0.333330005 0.833339989 0.000000000<br>Cu 0.005080000 0.833310008 0.198689997<br>Cu 0.166669995 0.833339989 0.097309999<br>Cu 0.335970014 0.832989991 0.299169987<br>Cu 0.500000000 0.000000000 0.048650000<br>Cu 0.832910001 0.999939978 0.148920000<br>Cu 0.671949983 0.000800000 0.253410012<br>Cu 0.501770020 0.994390011 0.343190014<br>Cu 0.833329976 0.166669995 0.000000000<br>Cu 0.505919993 0.168390006 0.199929997<br>Cu 0.666670024 0.166669995 0.097309999<br>Cu 0.839079976 0.166940004 0.299499989<br>Cu 0.500000000 0.333330005 0.048650000<br>Cu 0.835489988 0.333429992 0.146950006<br>Cu 0.676329970 0.333909988 0.247730002<br>Cu 0.833329976 0.500000000 0.000000000<br>Cu 0.506020010 0.498219997 0.199640006<br>Cu 0.666670024 0.500000000 0.097309999<br>Cu 0.838259995 0.499709994 0.300839990<br>Cu 0.500000000 0.666670024 0.048650000<br>Cu 0.832780004 0.666530013 0.149079993<br>Cu 0.672119975 0.665989995 0.254009992<br>Cu 0.502650023 0.671790004 0.343279988<br>Cu 0.833329976 0.833339989 0.000000000<br>Cu 0.505639970 0.833280027 0.196640000<br>Cu 0.666670024 0.833339989 0.097309999<br>Cu 0.838020027 0.833209991 0.300870001<br>Mn 0.518819988 0.333339989 0.361730009<br>C 0.675440013 0.213139996 0.519309998<br>H 0.605369985 0.154420003 0.550459981<br>H 0.730359972 0.261390001 0.570039988<br>H 0.715240002 0.117080003 0.476929992<br>H 0.697539985 0.406800002 0.432949990<br>O 0.636839986 0.359479994 0.467139989 |
| <b>CH<sub>3</sub>CO</b> | Cu 0.000000000 0.000000000 0.048650000<br>Cu 0.334080011 0.001130000 0.148300007<br>Cu 0.173089996 0.000750000 0.251580000<br>Cu 0.004820000 0.999870002 0.344040006<br>Cu 0.333330005 0.166669995 0.000000000<br>Cu 0.005620000 0.166730002 0.198449999                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |

|  |                |             |             |
|--|----------------|-------------|-------------|
|  | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|  | Cu 0.340570003 | 0.169599995 | 0.300449997 |
|  | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|  | Cu 0.333559990 | 0.332650006 | 0.148350000 |
|  | Cu 0.173419997 | 0.333860010 | 0.252579987 |
|  | Cu 0.004930000 | 0.333209991 | 0.344090015 |
|  | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|  | Cu 0.005880000 | 0.500050008 | 0.198599994 |
|  | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|  | Cu 0.340319991 | 0.500180006 | 0.297879994 |
|  | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|  | Cu 0.333270013 | 0.666630030 | 0.148120001 |
|  | Cu 0.172499999 | 0.667159975 | 0.252160013 |
|  | Cu 0.004870000 | 0.666469991 | 0.344469994 |
|  | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|  | Cu 0.005520000 | 0.833549976 | 0.198530003 |
|  | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|  | Cu 0.338779986 | 0.833079994 | 0.297670007 |
|  | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|  | Cu 0.832530022 | 0.000160000 | 0.148900002 |
|  | Cu 0.671869993 | 0.000220000 | 0.254049987 |
|  | Cu 0.503180027 | 0.997749984 | 0.343750000 |
|  | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|  | Cu 0.505859971 | 0.168870002 | 0.200210005 |
|  | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|  | Cu 0.838230014 | 0.166639999 | 0.300449997 |
|  | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|  | Cu 0.834529996 | 0.333279997 | 0.147420004 |
|  | Cu 0.674820006 | 0.333099991 | 0.248799995 |
|  | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|  | Cu 0.506049991 | 0.499430001 | 0.200020000 |
|  | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|  | Cu 0.838609993 | 0.499720007 | 0.299950004 |
|  | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|  | Cu 0.833829999 | 0.666790009 | 0.148090005 |
|  | Cu 0.673550010 | 0.666159987 | 0.250889987 |
|  | Cu 0.509019971 | 0.672930002 | 0.350089997 |
|  | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|  | Cu 0.505720019 | 0.830569983 | 0.198390007 |
|  | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|  | Cu 0.838440001 | 0.833150029 | 0.300190002 |
|  | Mn 0.516539991 | 0.332509995 | 0.362489998 |
|  | C 0.573249996  | 0.716250002 | 0.539129972 |
|  | C 0.546589971  | 0.589079976 | 0.467379987 |

|                          |                |             |             |
|--------------------------|----------------|-------------|-------------|
|                          | H 0.506219983  | 0.807319999 | 0.547360003 |
|                          | H 0.641579986  | 0.795520008 | 0.517660022 |
|                          | H 0.591099977  | 0.649619997 | 0.601540029 |
|                          | O 0.549539983  | 0.428999990 | 0.486970007 |
| <b>CH<sub>3</sub>CHO</b> | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|                          | Cu 0.333750010 | 0.000270000 | 0.148330003 |
|                          | Cu 0.172509998 | 0.999769986 | 0.251130015 |
|                          | Cu 0.005530000 | 0.999660015 | 0.344790012 |
|                          | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|                          | Cu 0.005340000 | 0.166500002 | 0.199169993 |
|                          | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|                          | Cu 0.339419991 | 0.167270005 | 0.301079988 |
|                          | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|                          | Cu 0.334410012 | 0.333220005 | 0.149499997 |
|                          | Cu 0.173690006 | 0.333110005 | 0.251929998 |
|                          | Cu 0.005920000 | 0.332980007 | 0.344720006 |
|                          | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|                          | Cu 0.005340000 | 0.499709994 | 0.199159995 |
|                          | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|                          | Cu 0.339540005 | 0.498869985 | 0.301189989 |
|                          | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|                          | Cu 0.333759993 | 0.666190028 | 0.148320004 |
|                          | Cu 0.172509998 | 0.666490018 | 0.251120001 |
|                          | Cu 0.005520000 | 0.666310012 | 0.344770014 |
|                          | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|                          | Cu 0.004760000 | 0.833119988 | 0.199129999 |
|                          | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|                          | Cu 0.337540001 | 0.833140016 | 0.299679995 |
|                          | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|                          | Cu 0.833199978 | 0.000000000 | 0.148719996 |
|                          | Cu 0.672429979 | 0.000970000 | 0.252189994 |
|                          | Cu 0.504660010 | 0.995620012 | 0.343470007 |
|                          | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|                          | Cu 0.505940020 | 0.168410003 | 0.200379997 |
|                          | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|                          | Cu 0.838460028 | 0.166329995 | 0.301019996 |
|                          | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|                          | Cu 0.833949983 | 0.333160013 | 0.148249999 |
|                          | Cu 0.674120009 | 0.333119988 | 0.250999987 |
|                          | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|                          | Cu 0.505930007 | 0.497979999 | 0.200399995 |
|                          | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|                          | Cu 0.838419974 | 0.499689996 | 0.300999999 |
|                          | Cu 0.500000000 | 0.666670024 | 0.048650000 |



|                                      |                |             |             |
|--------------------------------------|----------------|-------------|-------------|
|                                      | Cu 0.833190024 | 0.666360021 | 0.148719996 |
|                                      | Cu 0.672410011 | 0.665289998 | 0.252189994 |
|                                      | Cu 0.504610002 | 0.670549989 | 0.343529999 |
|                                      | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|                                      | Cu 0.504840016 | 0.833199978 | 0.197730005 |
|                                      | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|                                      | Cu 0.838190019 | 0.833019972 | 0.301099986 |
|                                      | Mn 0.515579998 | 0.332940012 | 0.362839997 |
|                                      | C 0.370419979  | 0.307550013 | 0.569679976 |
|                                      | C 0.487749994  | 0.330569983 | 0.566770017 |
|                                      | H 0.333869994  | 0.421720028 | 0.601899981 |
|                                      | H 0.350510001  | 0.194959998 | 0.611630023 |
|                                      | H 0.336210012  | 0.290650010 | 0.503669977 |
|                                      | H 0.530779958  | 0.342010021 | 0.630119979 |
|                                      | O 0.542219996  | 0.339460015 | 0.498320013 |
| <b>CH<sub>3</sub>CH<sub>2</sub>O</b> | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|                                      | Cu 0.334289998 | 0.000610000 | 0.147870004 |
|                                      | Cu 0.173500001 | 0.000470000 | 0.250910014 |
|                                      | Cu 0.005710000 | 0.000110000 | 0.344110012 |
|                                      | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|                                      | Cu 0.005830000 | 0.166639999 | 0.198449999 |
|                                      | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|                                      | Cu 0.340290010 | 0.169709995 | 0.299699992 |
|                                      | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|                                      | Cu 0.333519995 | 0.333009988 | 0.148110002 |
|                                      | Cu 0.173079997 | 0.333689988 | 0.252270013 |
|                                      | Cu 0.005220000 | 0.333550006 | 0.344319999 |
|                                      | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|                                      | Cu 0.005870000 | 0.500129998 | 0.198400006 |
|                                      | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|                                      | Cu 0.339830011 | 0.500230014 | 0.296860009 |
|                                      | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|                                      | Cu 0.333420008 | 0.666620016 | 0.147780001 |
|                                      | Cu 0.172319993 | 0.667379975 | 0.251610011 |
|                                      | Cu 0.005050000 | 0.666719973 | 0.344419986 |
|                                      | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|                                      | Cu 0.005340000 | 0.833800018 | 0.198280007 |
|                                      | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|                                      | Cu 0.338750005 | 0.832960010 | 0.297670007 |
|                                      | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|                                      | Cu 0.832369983 | 0.000270000 | 0.149230003 |
|                                      | Cu 0.671999991 | 0.000850000 | 0.254480004 |
|                                      | Cu 0.502569973 | 0.998340011 | 0.343870014 |
|                                      | Cu 0.833329976 | 0.166669995 | 0.000000000 |

|                           |                |             |             |
|---------------------------|----------------|-------------|-------------|
|                           | Cu 0.506049991 | 0.168709993 | 0.200149998 |
|                           | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|                           | Cu 0.838810027 | 0.166859999 | 0.300610006 |
|                           | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|                           | Cu 0.835150003 | 0.333110005 | 0.147259995 |
|                           | Cu 0.675559998 | 0.332569987 | 0.247899994 |
|                           | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|                           | Cu 0.506349981 | 0.498849988 | 0.200900003 |
|                           | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|                           | Cu 0.839089990 | 0.500090003 | 0.299650013 |
|                           | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|                           | Cu 0.833720028 | 0.666880012 | 0.148210004 |
|                           | Cu 0.673720002 | 0.667029977 | 0.250270009 |
|                           | Cu 0.507510006 | 0.676540017 | 0.350070000 |
|                           | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|                           | Cu 0.505789995 | 0.830169976 | 0.199450001 |
|                           | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|                           | Cu 0.838769972 | 0.833570004 | 0.300359994 |
|                           | Cu 0.517530024 | 0.328339994 | 0.363460004 |
|                           | C 0.484939992  | 0.623430014 | 0.590210021 |
|                           | C 0.576879978  | 0.554409981 | 0.534950018 |
|                           | H 0.450590014  | 0.740719974 | 0.559769988 |
|                           | H 0.512619972  | 0.657180011 | 0.656819999 |
|                           | H 0.421459973  | 0.525340021 | 0.595899999 |
|                           | H 0.641009986  | 0.652249992 | 0.530189991 |
|                           | H 0.611449957  | 0.436890006 | 0.565370023 |
|                           | O 0.542710006  | 0.511489987 | 0.447770000 |
| <b>CH<sub>3</sub>CHOH</b> | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|                           | Cu 0.334210008 | 0.001050000 | 0.148159996 |
|                           | Cu 0.173050001 | 0.000860000 | 0.251210004 |
|                           | Cu 0.005000000 | 0.999880016 | 0.344040006 |
|                           | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|                           | Cu 0.005570000 | 0.166850001 | 0.198550001 |
|                           | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|                           | Cu 0.340290010 | 0.169719994 | 0.300559998 |
|                           | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|                           | Cu 0.333510011 | 0.332489997 | 0.148530006 |
|                           | Cu 0.172940001 | 0.333790004 | 0.252799988 |
|                           | Cu 0.004620000 | 0.333380014 | 0.344309986 |
|                           | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|                           | Cu 0.005950000 | 0.500159979 | 0.198540002 |
|                           | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|                           | Cu 0.339069992 | 0.500169992 | 0.297569990 |
|                           | Cu 0.000000000 | 0.666670024 | 0.048650000 |

|                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
|-------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                                     | Cu 0.333380014 0.666670024 0.148130000<br>Cu 0.172330007 0.667649984 0.251960009<br>Cu 0.004760000 0.666419983 0.344489992<br>Cu 0.333330005 0.833339989 0.000000000<br>Cu 0.005370000 0.833580017 0.198440000<br>Cu 0.166669995 0.833339989 0.097309999<br>Cu 0.338470012 0.833869994 0.297769994<br>Cu 0.500000000 0.000000000 0.048650000<br>Cu 0.832499981 0.000220000 0.148920000<br>Cu 0.672029972 0.000110000 0.253890008<br>Cu 0.503189981 0.998459995 0.343710005<br>Cu 0.833329976 0.166669995 0.000000000<br>Cu 0.506070018 0.168620005 0.199949995<br>Cu 0.666670024 0.166669995 0.097309999<br>Cu 0.838259995 0.166569993 0.300660014<br>Cu 0.500000000 0.333330005 0.048650000<br>Cu 0.834850013 0.333200008 0.147170007<br>Cu 0.675509989 0.332850009 0.248610005<br>Cu 0.833329976 0.500000000 0.000000000<br>Cu 0.505959988 0.499069989 0.199949995<br>Cu 0.666670024 0.500000000 0.097309999<br>Cu 0.838779986 0.499769986 0.299470007<br>Cu 0.500000000 0.666670024 0.048650000<br>Cu 0.833419979 0.666719973 0.148289993<br>Cu 0.672789991 0.665889978 0.251509994<br>Cu 0.506770015 0.671209991 0.351760000<br>Cu 0.833329976 0.833339989 0.000000000<br>Cu 0.505639970 0.830020010 0.199190006<br>Cu 0.666670024 0.833339989 0.097309999<br>Cu 0.838469982 0.833079994 0.300110012<br>Mn 0.516740024 0.336690009 0.359770000<br>C 0.633440018 0.635429978 0.515550017<br>C 0.525110006 0.592459977 0.477569997<br>H 0.697189987 0.561049998 0.483069986<br>H 0.636449993 0.608370006 0.586910009<br>H 0.650969982 0.774030030 0.504840016<br>H 0.460669994 0.662729979 0.511340022<br>H 0.431059986 0.386860013 0.511380017<br>O 0.505739987 0.401730001 0.494949996 |
| <b>C<sub>2</sub>H<sub>5</sub>OH</b> | Cu 0.000000000 0.000000000 0.048650000<br>Cu 0.333510011 0.000390000 0.148660004<br>Cu 0.172680005 0.000690000 0.251769990<br>Cu 0.004900000 0.000440000 0.344500005<br>Cu 0.333330005 0.166669995 0.000000000                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |

|  |                |             |             |
|--|----------------|-------------|-------------|
|  | Cu 0.006070000 | 0.166779995 | 0.198770002 |
|  | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|  | Cu 0.340640008 | 0.168970004 | 0.301160008 |
|  | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|  | Cu 0.333099991 | 0.333359987 | 0.148920000 |
|  | Cu 0.173360005 | 0.333359987 | 0.253259987 |
|  | Cu 0.004550000 | 0.333579987 | 0.344880015 |
|  | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|  | Cu 0.005930000 | 0.500029981 | 0.198780000 |
|  | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|  | Cu 0.340939999 | 0.497469991 | 0.301360011 |
|  | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|  | Cu 0.333499998 | 0.666109979 | 0.148680001 |
|  | Cu 0.172729999 | 0.665719986 | 0.251729995 |
|  | Cu 0.004960000 | 0.666670024 | 0.344460011 |
|  | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|  | Cu 0.005450000 | 0.833350003 | 0.198689997 |
|  | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|  | Cu 0.336290002 | 0.833050013 | 0.299369991 |
|  | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|  | Cu 0.832960010 | 0.000250000 | 0.149059996 |
|  | Cu 0.672330022 | 0.000580000 | 0.253589988 |
|  | Cu 0.501959980 | 0.994790018 | 0.342379987 |
|  | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|  | Cu 0.506179988 | 0.168599993 | 0.199599996 |
|  | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|  | Cu 0.838689983 | 0.167600006 | 0.300570011 |
|  | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|  | Cu 0.835709989 | 0.333389997 | 0.146840006 |
|  | Cu 0.676710010 | 0.333550006 | 0.247390002 |
|  | Cu 0.833329976 | 0.500000000 | 0.000000000 |
|  | Cu 0.506110013 | 0.498250008 | 0.200080007 |
|  | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|  | Cu 0.838509977 | 0.499729991 | 0.300870001 |
|  | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|  | Cu 0.832790017 | 0.666570008 | 0.149169996 |
|  | Cu 0.672169983 | 0.665889978 | 0.254200011 |
|  | Cu 0.502409995 | 0.672429979 | 0.343670011 |
|  | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|  | Cu 0.505890012 | 0.833010018 | 0.196620002 |
|  | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|  | Cu 0.838389993 | 0.833599985 | 0.300770015 |
|  | Cu 0.519129992 | 0.333090007 | 0.362150013 |
|  | Mn 0.560609996 | 0.144649997 | 0.572910011 |

|                                   |                |             |             |
|-----------------------------------|----------------|-------------|-------------|
|                                   | C 0.662570000  | 0.199349999 | 0.527469993 |
|                                   | H 0.502499998  | 0.092660002 | 0.525129974 |
|                                   | H 0.523980021  | 0.254880011 | 0.607739985 |
|                                   | H 0.577610016  | 0.041719999 | 0.621140003 |
|                                   | H 0.721689999  | 0.247700006 | 0.575070024 |
|                                   | H 0.698019981  | 0.091779999 | 0.489529997 |
|                                   | H 0.702929974  | 0.367190003 | 0.431100011 |
|                                   | O 0.638499975  | 0.342680007 | 0.466800004 |
| <b>C<sub>2</sub>H<sub>6</sub></b> | Cu 0.000000000 | 0.000000000 | 0.048650000 |
|                                   | Cu 0.333620012 | 0.000180000 | 0.148739994 |
|                                   | Cu 0.172839999 | 0.000240000 | 0.251709998 |
|                                   | Cu 0.005790000 | 0.000100000 | 0.344940007 |
|                                   | Cu 0.333330005 | 0.166669995 | 0.000000000 |
|                                   | Cu 0.005910000 | 0.166710004 | 0.198980004 |
|                                   | Cu 0.166669995 | 0.166669995 | 0.097309999 |
|                                   | Cu 0.339879990 | 0.167630002 | 0.301640004 |
|                                   | Cu 0.000000000 | 0.333330005 | 0.048650000 |
|                                   | Cu 0.333510011 | 0.333310008 | 0.149140000 |
|                                   | Cu 0.173730001 | 0.333270013 | 0.252840012 |
|                                   | Cu 0.005950000 | 0.333420008 | 0.344989985 |
|                                   | Cu 0.333330005 | 0.500000000 | 0.000000000 |
|                                   | Cu 0.005920000 | 0.499940008 | 0.198990002 |
|                                   | Cu 0.166669995 | 0.500000000 | 0.097309999 |
|                                   | Cu 0.339870006 | 0.498640001 | 0.301930010 |
|                                   | Cu 0.000000000 | 0.666670024 | 0.048650000 |
|                                   | Cu 0.333550006 | 0.666379988 | 0.148739994 |
|                                   | Cu 0.172830001 | 0.666230023 | 0.251749992 |
|                                   | Cu 0.005760000 | 0.666750014 | 0.344940007 |
|                                   | Cu 0.333330005 | 0.833339989 | 0.000000000 |
|                                   | Cu 0.005290000 | 0.833360016 | 0.198799998 |
|                                   | Cu 0.166669995 | 0.833339989 | 0.097309999 |
|                                   | Cu 0.336979985 | 0.833079994 | 0.299910009 |
|                                   | Cu 0.500000000 | 0.000000000 | 0.048650000 |
|                                   | Cu 0.832560003 | 0.000150000 | 0.149250001 |
|                                   | Cu 0.672270000 | 0.001090000 | 0.254819989 |
|                                   | Cu 0.503269970 | 0.995199978 | 0.344929993 |
|                                   | Cu 0.833329976 | 0.166669995 | 0.000000000 |
|                                   | Cu 0.506389976 | 0.167400002 | 0.198970005 |
|                                   | Cu 0.666670024 | 0.166669995 | 0.097309999 |
|                                   | Cu 0.839139998 | 0.166859999 | 0.300909996 |
|                                   | Cu 0.500000000 | 0.333330005 | 0.048650000 |
|                                   | Cu 0.835399985 | 0.333339989 | 0.147220001 |
|                                   | Cu 0.676329970 | 0.333469987 | 0.248710006 |
|                                   | Cu 0.833329976 | 0.500000000 | 0.000000000 |

|  |                |             |             |
|--|----------------|-------------|-------------|
|  | Cu 0.506320000 | 0.499220014 | 0.198949993 |
|  | Cu 0.666670024 | 0.500000000 | 0.097309999 |
|  | Cu 0.839119971 | 0.500060022 | 0.300799996 |
|  | Cu 0.500000000 | 0.666670024 | 0.048650000 |
|  | Cu 0.832769990 | 0.666580021 | 0.149049997 |
|  | Cu 0.672360003 | 0.666000009 | 0.254119992 |
|  | Cu 0.503279984 | 0.670539975 | 0.344000012 |
|  | Cu 0.833329976 | 0.833339989 | 0.000000000 |
|  | Cu 0.506349981 | 0.833350003 | 0.197310001 |
|  | Cu 0.666670024 | 0.833339989 | 0.097309999 |
|  | Cu 0.838800013 | 0.833450019 | 0.300740004 |
|  | Cu 0.515799999 | 0.332500011 | 0.356099993 |
|  | Mn 0.602209985 | 0.409269989 | 0.547710001 |
|  | C 0.613240004  | 0.606750011 | 0.555859983 |
|  | H 0.658760011  | 0.356200010 | 0.498899996 |
|  | H 0.520269990  | 0.372310013 | 0.528249979 |
|  | H 0.617689967  | 0.342079997 | 0.610400021 |
|  | H 0.556810021  | 0.660070002 | 0.604260027 |
|  | H 0.598649979  | 0.672720015 | 0.492399991 |
|  | H 0.694450021  | 0.643299997 | 0.576120019 |