Electronic Supplementary Information for Dalton Transactions


**Molecular modelling for coordination compounds: Cu(II)–amine complexes**

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**Table ESI1: Comparison of LFMM and X-ray structural data for training set: Individual Cu-N bond length differences (column 2), Overall Cu-N rms deviations (column 3) and rms heavy atom overlay deviation (column 4).**

| Refcode | M-L(LFMM-Xray) | M-L(rms) | Heavy Atom rmsd |
|---|---|---|---|
| RUMPUK | -0.020644702<br>-0.025496941<br>-0.021363594<br>-0.025988711 | 0.023495287 | 0.21624368 |
| GUGWOU | -0.013054539<br>-0.023978375<br>-0.013449652<br>-0.024627885 | 0.019575555 | 0.06527555 |
| ZENDOL | 0.018035818<br>-0.011686556<br>0.018066779<br>-0.012180776 | 0.015302338 | 0.13880637 |
| CEFBEU | -0.00034431831<br>0.0020495702<br>-0.0003066934<br>0.0028932348 | 0.0017877473 | 0.085605033 |
| DEENCU01 | 0.015891517<br>0.0095793363<br>0.015856655<br>0.0095277708 | 0.013100724 | 0.12976283 |
| DMEDCU | -0.033980723<br>0.011588046<br>-0.03385349<br>0.011665562 | 0.025353089 | 0.07828071 |
| DUFSAY | -0.007769973<br>-0.00095531723<br>0.0075342963<br>0.0094053 | 0.0071852347 | 0.2312602 |
| PRACUS10 | 0.0069301459<br>0.010029283<br>0.0062009706<br>0.010153456 | 0.0085170148 | 0.12462682 |
| ABUCUP01 | 0.006423282<br>-0.0045041228<br>0.0063923988<br>-0.0044982978 | 0.0055372179 | 0.1079006 |
| CHXCUB01 | 0.021260671<br>0.021081386<br>0.021268543<br>0.021089254 | 0.021175154 | 0.16609316 |
| HAFTAJ | 0.027064983<br>0.0060049938<br>0.027057892<br>0.00600811 | 0.019601021 | 0.14256807 |
| DEPLEP | 0.026566431<br>0.015723232<br>0.026348511<br>0.015651852 | 0.021749826 | 0.15478942 |
| LOPMOS | 0.012753584<br>-0.00020912768<br>0.0042377403<br>0.015015078<br>0.016714998 | 0.011708969 | 0.091193303 |

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|---|---|---|---|
| JIBZUP | -0.0013472351<br>0.027050892<br>-0.015975691<br>0.00033881731<br>0.011081458 | 0.014911083 | 0.11984482 |
| KIQNAZ | 0.010520567<br>0.0082179662<br>-0.079845905<br>0.011658964<br>0.007171371<br>-0.080906518 | 0.047058139 | 0.041382059 |
| FUPJEF | -0.10968667<br>0.025775608<br>0.030529261<br>-0.10969266<br>0.025722004<br>0.03057115 | 0.067399651 | 0.056505885 |
| LOMREK | 0.017774582<br>0.036790013<br>-0.1210169<br>0.035424463<br>0.017593531<br>-0.12032929 | 0.073437154 | 0.060480036 |
| TACCUP | 0.0044373027<br>0.0035049594<br>0.0038806244<br>-0.076627553<br>0.0048840647<br>-0.075684361 | 0.044103652 | 0.073759377 |

**Table ESI2: CSD refcodes for structures containing isolated $[Cu(en)_2]^{2+}$**

AENNIC10
BETDCU01
BEZLIB
CEDHAU
DADTOR01
EDCOPT
GASRUN
GEDJOO
GUGWOU
HACBAP
JIRCIW
QEPTIO
SEVNUC
XEPGII
EKABAT
OHUQUD

**Table ESI31: Comparison of LFMM and X-ray structural data for molecules NOT in the training set: Overall Cu-N rms deviations (column 2) and rms heavy atom overlay deviation (column 3).**

| Refcode | M-L(rms) | Heavy Atom rmsd |
|---|---|---|
| FUVWUO | 0.0041616568 | 0.048090417 |
| ETEACU | 0.0066103977 | 0.050595842 |
| ECUTAR | 0.0067533781 | 0.2871125 |
| BASPAN | 0.0071031465 | 0.073318467 |
| DIXZOZ | 0.0073405053 | 0.10687778 |
| NEPXUB | 0.0075804829 | 0.18013251 |
| TMENCW | 0.0093264328 | 0.073416159 |

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|---|---|---|
| BAPTOB | 0.011256737 | 0.34053084 |
| MUMQOA | 0.012592877 | 0.045391757 |
| DESKIV | 0.013415923 | 0.46261939 |
| NEPYAI | 0.016608953 | 0.34501559 |
| HXPACU | 0.01771294 | 0.099270113 |
| XPACUT | 0.018856583 | 0.066976033 |
| LIVBOH | 0.022456337 | 0.17734326 |
| RABZEV | 0.025522094 | 0.099637575 |
| XOTYOU | 0.025855331 | 0.094532721 |
| HENCUC | 0.02596858 | 0.23569834 |
| KUKFOL | 0.026786551 | 0.076940075 |
| CMENOX | 0.027756978 | 0.059818897 |
| IGOWIK | 0.028513007 | 0.16795373 |
| VAZBUT | 0.029122991 | 0.064148106 |
| AJAROS | 0.02918965 | 0.17646572 |
| VAZBUT10 | 0.029760977 | 0.064119652 |
| IGOWEG | 0.029807214 | 0.19979657 |
| HMTZCP | 0.030359533 | 0.33133802 |
| AJEVUG | 0.031730711 | 0.15501606 |
| SEVGIJ | 0.032454703 | 0.13079427 |
| IGOWAC | 0.032745406 | 0.18524019 |
| MHMZCU | 0.034325615 | 0.15664057 |
| COZCOJ | 0.036156949 | 1.0643948 |
| SINLAC | 0.036687128 | 0.075745039 |
| ACUYAY | 0.039863739 | 0.14496507 |
| NENCOY | 0.040466934 | 0.10011022 |
| BULQAA | 0.040589251 | 0.25383174 |
| ZADSEC | 0.041835606 | 0.15587354 |
| GANHEI | 0.044141691 | 0.18384753 |
| VOPSEY | 0.045060605 | 0.11642365 |
| HAFSUC | 0.046731781 | 0.040917836 |
| CAKQOV | 0.051748451 | 0.054183509 |
| BAMYIY | 0.052774791 | 1.0338836 |
| NELHAN | 0.054425247 | 0.14148597 |
| FUPJAB | 0.056059346 | 0.1185255 |
| ECIYAQ | 0.058430515 | 0.099873632 |
| JETDOB | 0.059762213 | 0.12109806 |
| VUTTUZ01 | 0.06226296 | 0.059331179 |
| VIFKAW | 0.065872028 | 0.14658365 |
| ZALFUN | 0.07564605 | 0.088481456 |
| ZURZOB | 0.081257172 | 0.072823979 |
| RAZJEH | 0.081686661 | 0.16286021 |
| PEDJEN01 | 0.083342664 | 0.15626127 |
| VIFDIX | 0.083818391 | 0.34697205 |
| EFAJOK | 0.086292207 | 0.17010167 |
| QAGSUN | 0.09394329 | 0.19587229 |
| ZURZIV | 0.094735622 | 0.12016786 |
| JUFLUR | 0.095631234 | 0.18154001 |
| ETACUB | 0.09740378 | 0.16714506 |
| DIRJET | 0.097407795 | 0.10819291 |
| PIWTAQ | 0.10070819 | 0.21282169 |
| JOKKUP | 0.10527982 | 0.096392341 |
| ZIWGUH | 0.1097803 | 0.24405496 |
| RAZJAD | 0.11622385 | 0.21523662 |
| CIQKES | 0.11857644 | 0.17482522 |
| AMECUA | 0.12202942 | 0.15234369 |
| FENRAR | 0.12382247 | 0.28066605 |
| QAGCAD | 0.12594959 | 0.20158324 |
| MIRXAM | 0.13132821 | 0.2733683 |

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|---|---|---|
| XIXRIF | 0.13547194 | 0.26139906 |