

Supporting Information

On the nature of spin- and orbital-resolved Cu^+ - NO charge transfer
in the Gas Phase and at Cu(I) Sites in ZeolitesP. Kozyra¹, M. Radon¹, J. Datka¹ and E. Broclawik^{2*}¹ Faculty of Chemistry, Jagiellonian University, ul. Ingardena 3, 30-060 Krakow, Poland² Jerzy Haber Institute of Catalysis PAS, ul. Niezapominajek 8, 30-239 Krakow, PolandRECEIVED DATE (...); E-mail: broclawi@chemia.uj.edu.pl**Contents**

1. Cartesian coordinates of studied molecular models

S1

Cartesian coordinates of studied models

[CuNO]⁺ - a bare Cu⁺ cation and NO molecule

\$coord

-1.42534228065848	0.05701215183947	0.00000000000000	cu
2.05800910400446	-0.75887749597859	0.00000000000000	n
3.85891548407945	0.43794250378411	0.00000000000000	o

(T1)CuNO - Cu⁺ cation linked to an [Al(OH)₄]⁻ anion (T1)

\$coord

5.17500202641716	-0.25906551764128	0.00000000000000	n
7.11561480060141	0.82585441888721	0.00000000000000	o
1.85164603769995	-0.30758719200408	0.00000000000000	cu
-1.01614194343498	-0.55287482052831	-2.36765236163647	o
-1.01614194343498	-0.55287482052831	2.36765236163647	o
-6.03939167598191	-1.87523569760549	0.00000000000000	o
-3.47229921387899	0.13481373637489	0.00000000000000	al
-4.20603338644983	3.32263661589988	0.00000000000000	o
-5.96760763299992	3.80554462811580	0.00000000000000	h
-5.81606885629325	-3.68635762436500	0.00000000000000	h
-0.98338609580027	0.36496065316132	-3.94874489846685	h
-0.98338609580027	0.36496065316132	3.94874489846685	h

(M7)CuNO - M7 cluster hosting Cu+ cation and NO molecule
\$coord

-0.62827931354394	2.41217561471769	0.00000000000000	o
-0.62827931354394	0.18590941942948	0.00000000000000	n
1.25655673736122	-2.59808503414717	0.00000000000000	cu
4.64844224350920	-6.75756617265306	-0.20872975861803	al
3.00744896235676	-4.84952805777333	-2.55082297029278	o
2.78586906242686	-5.24209231594431	2.27111885764663	o
4.12134456470959	-9.95693577495593	-0.62840592523039	o
1.69250911972639	-5.40264349327614	-5.34591011938424	si
2.63635010935659	-5.58336561301429	5.38443030769323	si
1.81235936417954	-11.96027091574982	-0.61312370570259	si
-3.04298527226407	-7.61362557930988	5.91124263776665	si
-4.03755975362953	-7.13577417736135	-4.87957282199648	si
3.64215523628330	-3.03065669551133	6.84672914581747	o
4.61349552832090	-7.98555402231533	5.96599746784186	o
7.79812715237505	-5.92939346236967	0.08461818053867	o
2.13165325042624	-13.89294539714174	1.85133497661444	o
1.63696060445251	-13.68497719836911	-3.22729409320956	o
-0.90040751199608	-10.42517602709384	-0.31324298147013	o
2.74226739911968	-8.15279672176266	-6.45469212138561	o
-3.78466141370527	-7.74703839202705	2.90906979225441	o
-1.38543609581262	-5.47336273420469	-4.87863740729804	o
-5.54976060375709	-12.06930625450771	1.02716659713102	o
-3.80025732785922	-9.56894654503731	0.38890385762376	si
-3.36333362598900	-9.67818030509486	-6.56767131969024	o
-6.28658959630639	-5.36544611363161	-6.12654108626704	o
-5.18128469136587	-5.92300618624700	7.41623796012624	o
-0.25054374050153	-6.25094557197925	6.32623795143350	o
-2.85458897254541	-10.56082816590727	7.01244116666735	o
-4.92436312337500	-7.90331122819270	-1.99242574876545	o
2.49257025616341	-3.17913629891666	-7.37053681049591	o
2.02456810958510	-1.79110371866838	-8.46179537714655	h
3.70760591927398	-9.12167847941103	-7.66543054606335	h
-6.63907086221765	-4.07417698718837	-7.36947289438435	h
-3.55892411511565	-11.32458198395826	-7.33422571265655	h
3.40864360219999	-1.52191971435799	7.84957118133579	h
-5.49030035428973	-4.54868924212248	8.57910582896394	h
-2.53224317773715	-11.58494285447672	8.49020363807910	h
-6.14678761773989	-13.77750766444789	0.77795511392727	h
5.42622917176342	-8.88234081802412	7.33411421878341	h
2.12084023445763	-15.56617930490033	2.58391775335084	h
1.65574259776114	-14.08202199845927	-5.01013214745174	h
9.39099098513454	-5.21551331042204	-0.42868449361732	h