様　式　Ｃ－１９、Ｆ－１９－１、Ｚ－１９　（共通）

科学研究費助成事業　　研究成果報告書

令和　２ 年　 ６ 月　 ３ 日現在

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研究種目：基盤研究(B)（一般）
研究期間：2017～2019
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研究課題名（和文）Synthesis, Characterization and Testing of N-Heterocyclic Carbene-modified Magic Number Metallic Clusters for C-H Oxidation Catalysis

研究課題名（英文）Synthesis, Characterization and Testing of N-Heterocyclic Carbene-modified Magic Number Metallic Clusters for C-H Oxidation Catalysis

研究代表者

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研究成果の概要（和文）：本研究では触媒としての機能開拓を目指し、ホスフィンとN-ヘテロサイクリックカルベン配位子を有する新規金ナノクラスターの合成に初めて成功した。今回得られた金ナノクラスターはホスフィンのみからなる金ナノクラスターと比較して高い安定性を示すだけでなく、CO2の還元やベンジルアルコールの選択的酸化に対する触媒活性を示した。また合成手法やNHCの性質をチューニングすることで、NHCのみからなる金ナノクラスターの合成にも成功した。

研究成果の学術的意義や社会的意義
The development of NHC gold clusters will open up previously unknown possibilities in catalysis. Since the NHC not only forms a stable bond to the cluster, but also stabilizes the cluster itself, we will be able to perform the surgical removal of specific ligands without cluster collapse.

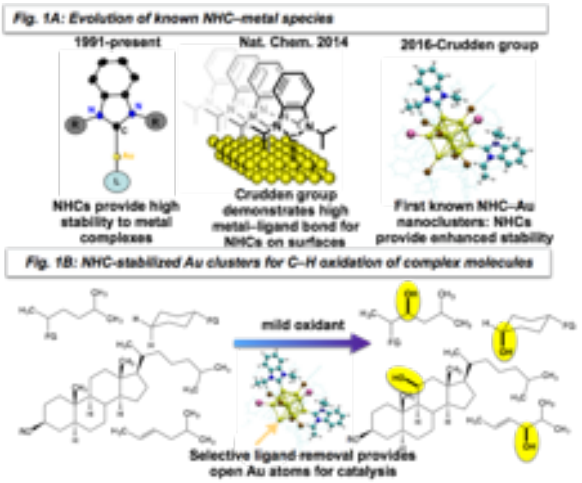
研究成果の概要（英文）：With the Kakenhi funds, we have made significant progress on the synthesis and characterization of novel gold nanoclusters bearing phosphine and N-Heterocyclic carbenes (NHC) ligands. In addition, we have made strides to understanding their properties in terms of stability and catalytic reactivity. These results are broken down by cluster type. By tuning the method of synthesis and nature of the NHC, we have prepared new NHC-based gold clusters.

研究分野：Organometallic Chemistry

キーワード：Nano Materials　Nanocluster　N-Heterocyclic Carbene　Gold　CO2 Reduction　C-H Oxidation

１．研究開始当初の背景

N-Heterocyclic carbenes (NHC) have been employed as ligands for transition metal complexes for decades. They provide stable, oxidation-resistant bonds to the metal that enable the use of metal complexes as catalyst precursors under conditions where related phosphine ligated-catalysts would be unstable. Our group was the first to demonstrate that NHCs are also exceptional ligands for metal surfaces. We have shown that NHCs form exceptionally strong bonds to Au surfaces that are resistant to heat, pH extremes, and oxidation (Fig 1A). NHCs remain intact on the surface until 600K, which gives an estimate of the bond strength at 158±10 kJ/mol, compared with 125 kJ/mol for thiols.



In unpublished work, we have extrapolated these results to magic number Au nanoclusters. Unlike nanoparticles, which are imperfect composite materials made up of a distribution of species centered around one size, magic number nanoclusters are perfect molecular entities composed of a specific number of atoms. They are molecules. Since their properties are size dependent, they are also nanomaterials. The atomic precision of these species and their exceptionally high surface to core atom ratio makes nanoclusters extremely exciting in the area of catalysis.

Following up on the groundbreaking work of Haruta on gold nanoparticle catalysis, thiol-protected nanoclusters have been examined as catalysts for a variety of reactions, including the oxidation of CO to CO_2 using O_2, and the reduction of nitroarenes. Although there are cases where ligand-bound nanoclusters are employed directly as catalysts, there is considerable evidence that, at least in some processes, thiol ligands have to be removed because they block the surface too efficiently. For this reason, it is common to deposit the nanoclusters on support and then remove the ligands either oxidatively or thermally. Challenges with this process are: 1) ensuring that the unligated clusters do not migrate on the surface and agglomerate into larger, less active clusters; 2) keeping the same active faces/facets after deposition and calcination; 3) ensuring that mixed-metal species retain the same composition. Although there are some cases where these challenges are met, in many cases they are not. With our collaborator, Tatsuya Tsukuda, a world expert in the preparation and use of nanoclusters in catalysis, we will employ NHC-stabilized nanoclusters as highly efficient catalysts for the transformation of complex molecules. The selective oxidation of C–H bonds will be the goal (Fig 1B).

２．研究の目的

N-Heterocyclic carbenes (NHC) are exciting alternatives to thiols since they form strong bonds to metal surfaces, giving films that are resistant to heat, pH extremes, and oxidation. We have recently showed that NHCs also provide stability to "magic number" gold nanoclusters, which are unique molecular species bridging the gap between molecules and materials. Herein we propose to employ mixed NHC/phosphine Au clusters as novel catalysts for C–H oxidation reactions. Previous work with thiol-stabilized nanoclusters required removal of all ligands for activity, which decreases the ability to tune the catalyst. We plan to selectively remove phosphine ligands in mixed clusters to generate active sites for C–H oxidation. This reaction is important for late stage functionalization.

３．研究の方法

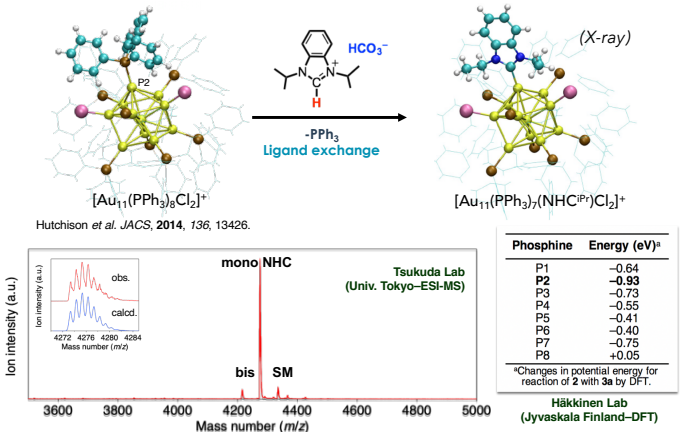
(1) Preparation of new mixed NHC/phosphine and investigation of the nature
(2) Investigation of catalytic activity
(3) Preparation of new all-NHC Au clusters

４．研究成果

(1) The use of NHCs to displace phosphines on known phosphine-stabilized clusters has been accomplished during this funding period. We began by preparing phosphine-stabilized undecagold clusters $Au_{11}(PPh_3)_7Cl_3$ and $[Au_{11}(PPh_3)_8Cl_2]Cl$ and treating these with di-isopropyl benzimidazolium hydrogen carbonate. The less stable cluster ($Au_{11}(PPh_3)_7Cl_3$) was not suitable but the more stable cluster gave predominantly a single NHC-containing cluster ($[Au_{11}(PPh_3)_7(NHC^{iPr})Cl_2]Cl$) after heating in THF at 66 °C. This cluster results from substitution of one phosphine ligand for the NHC. When the free NHC was employed, a complex mixture

resulting from displacement of multiple phosphines was obtained.

The structure of cluster $[Au_{11}(PPh_3)_7(NHC^{iPr})Cl_2]Cl$ was predicted by mass spectrometric analysis carried out in the Tsukuda lab and DFT work from collaborator Häkkinen. Eventually this was confirmed by a single crystal X-ray diffraction study carried out in the Tskuda lab, using a high purity sample prepared by ion exchange in our lab.

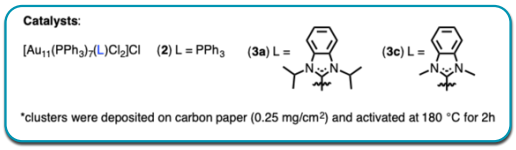


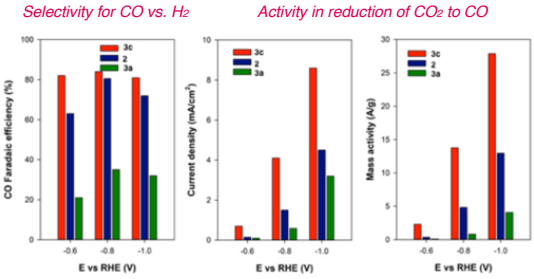
Phosphine	Energy (eV)[a]
P1	–0.64
P2	**–0.93**
P3	–0.73
P4	–0.55
P5	–0.41
P6	–0.40
P7	–0.75
P8	+0.05

[a]Changes in potential energy for reaction of **2** with **3a** by DFT.

Häkkinen Lab
(Jyvaskala Finland–DFT)

(2) Key to our progress in the use of these clusters as catalysts is understanding of the ligand exchange and displacement properties in order to create active sites for catalysis. We have made progress in understanding of these factors for the NHC-stabilized nanoclusters. The thermal loss of phosphine was assessed for all the clusters prepared by thermal gravimetric analysis (TGA). In all cases, phosphine loss was initiated at about 180 °C. Using this temperature as a starting point, we examined the behavior of the clusters in the electrocatalytic reduction of CO_2 to CO after heating of the clusters to 180 °C. As an indication that phosphine removal was key to catalytic activity, we also performed the catalysis after heating to only 50 °C and found significantly lower activity.





The most active of the clusters was cluster $[Au_{11}(PPh_3)_7(NHC^{Me})Cl_2]Cl$, in which the dimethyl NHC derivative is employed. This particular cluster out-performed the all phosphine cluster and also the other NHC–stabilized clusters examined. Interestingly, this particular cluster was also by far the most stable against decomposition to nanoparticles leading to the exciting conclusion that retaining the nanocluster structure was a key component of the catalytic activity. This cluster had the best catalytic activity, as assessed by current density and mass activity. It also was the most selective for CO vs H_2 production (Faradaic efficiency).

In order to further investigate the possibility that retaining the nanocluster form was critical to activity, we examined the effect of increasing the density of the nanocluster on the electrode. If nanoclusters that have lost a ligand undergo agglomeration to nanoparticles, we should expect to see a significant improvement as the amount of catalyst is increased since this will increase the likelihood of nanoparticle formation due to Ostwald ripening.

Current density was found to stay basically the same when the catalyst loading on the surface was quadrupled and CO mass activity actually decreased. This suggests that either there is multilayer deposition of the catalyst, (unlikely at 1 mg/cm^2 on a 1 cm^2 electrode), or that agglomeration into nanoparticles leads to lower activity, which is consistent with the fact that the most stable dimethyl NHC–nanocluster is also the most active.

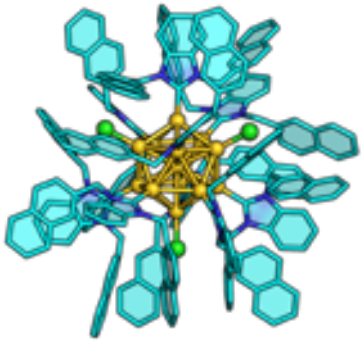
we worked to improve the yield of the clusters even further to permit us to carry out more experiments studying the ligand exchange behaviour and catalysis. With revised synthetic methods in hand, we then moved to examine phosphine dissociation in detail and catalytic C–H oxidation.

To obtain a better idea about phosphine dissociation under more controlled conditions, we are in the process of carrying out inversion transfer experiments with the NHC-protected clusters to shed light on the process of phosphine exchange. Since a single resonance is observed in the ^{31}P NMR, we know that there is some type of exchange going on, and if we can better understand this, we hope to exploit it in a catalytic system. These results are ongoing.

We have also carried out C–H oxidation studies with cluster $[Au_{11}(PPh_3)_7(NHC^{iPr})Cl_2]Cl$. Initially we used a simple substrate, benzyl alcohol, and looked for the absolute activity in terms of conversion to product and also selectivity for initial C–H oxidation to benzaldehyde vs. over oxidation to the corresponding benzyl ester. Our preliminary results with these gold clusters have shown that these give improved yields and selectivities compared with the corresponding all phosphine clusters. For example, under conditions where the all phosphine cluster gave a 2:1 ratio of benzaldehyde to the over oxidized benzylester, the NHC-containing cluster gave a 10:1

ratio and higher yields. Selectivity of up to 44:1 has been obtained but at lower yields.

(3) Building on the previous work, we strived to make a cluster in which the NHC ligand was the predominant ligand, not the ancillary ligand. To achieve this, we investigated the reduction of well-defined NHC–Au–Cl complexes. This produced clusters composed of an icosahedral Au_{13} core (similar to the abovementioned Au_{11}) which is an 8-electron superatom. These clusters represent the first examples of gold clusters larger than three atoms stabilized entirely by NHC and halide ligands. The direct reduction preparation was initially developed for NHCs bearing 1,3-disubstituted benzimidazolium ligands bearing benzyl wingtip groups. The procedure was found to be general, and $[Au_{13}(NHC)_9Cl_3]^{2+}$ clusters were prepared with a variety of benzimidazole- and triazole-derived NHC ligands. This synthetic success allowed us to study the effect of the structure of NHC ligands, including electronic configuration and steric effects on size, structure, and properties of gold nanoclusters. In particular, X-ray crystallography shows that the clusters with benzyl and naphthyl wingtips are characterized by multiple CH–π and π–π interactions, which rigidify the ligand shell and likely contribute to the exceptionally high photoluminescent quantum yields observed, up to 16.0%, which is significantly greater than that of the most luminescent gold clusters.



５．主な発表論文等

〔雑誌論文〕　計24件（うち査読付論文　24件／うち国際共著　24件／うちオープンアクセス　2件）

１．著者名 Chen Hao、Saunders John E.、Borjian Sogol、Wu Xiaowei、Crudden Cathleen M.、Xu Dan-Xia、Loock Hans-Peter	４．巻 3
２．論文標題 Tetrasulfide-Functionalized Mesoporous Silica on Nanowire Ring Resonators for Detection of Aqueous Lead, Pb(II)	５．発行年 2019年
３．雑誌名 Advanced Sustainable Systems	６．最初と最後の頁 1800084～1800084
掲載論文のDOI（デジタルオブジェクト識別子） 10.1002/adsu.201800084	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 Nambo Masakazu、Tahara Yasuyo、Yim Jacky C.‐H.、Crudden Cathleen M.	４．巻 25
２．論文標題 Cu‐Catalyzed Desulfonylative Amination of Benzhydryl Sulfones	５．発行年 2019年
３．雑誌名 Chemistry ? A European Journal	６．最初と最後の頁 1923～1926
掲載論文のDOI（デジタルオブジェクト識別子） 10.1002/chem.201805638	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 Smith Christene A.、Narouz Mina R.、Lummis Paul A.、Singh Ishwar、Nazemi Ali、Li Chien-Hung、Crudden Cathleen M.	４．巻 119
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３．雑誌名 Chemical Reviews	６．最初と最後の頁 4986～5056
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１．著者名 Torres‐Rocha Olga Lidia、Wu Xiaowei、Zhu Chunyang、Crudden Cathleen M.、Cunningham Michael F.	４．巻 -
２．論文標題 Synthesis of Diblock and Triblock Polymers from Cyclooctadiene and Norbornene Via ROMP in Miniemulsion	５．発行年 2019年
３．雑誌名 Macromolecular Rapid Communications	６．最初と最後の頁 1900087～1900087
掲載論文のDOI（デジタルオブジェクト識別子） 10.1002/marc.201900087	査読の有無 有
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1．著者名 Yan Dong-Mei、Crudden Cathleen M.、Chen Jia-Rong、Xiao Wen-Jing	4．巻 9
2．論文標題 A Career in Catalysis: Howard Alper	5．発行年 2019年
3．雑誌名 ACS Catalysis	6．最初と最後の頁 6467～6483
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2．論文標題 Modular synthesis of α-fluorinated arylmethanes via desulfonylative cross-coupling	5．発行年 2019年
3．雑誌名 Nature Communications	6．最初と最後の頁 4528
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3．雑誌名 Journal of the American Chemical Society	6．最初と最後の頁 14997～15002
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1．著者名 Yim Jacky C.-H.、Nambo Masakazu、Tahara Yasuyo、Crudden Cathleen M.	4．巻 48
2．論文標題 Copper-catalyzed Desulfonylative Cross-coupling of Benzhydryl Sulfones with Azoles	5．発行年 2019年
3．雑誌名 Chemistry Letters	6．最初と最後の頁 975～977
掲載論文のDOI（デジタルオブジェクト識別子） 10.1246/cl.190334	査読の有無 有
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1．著者名 Maekawa Yuuki、Ariki Zachary T.、Nambo Masakazu、Crudden Cathleen M.	4．巻 17
2．論文標題 Pyridine-catalyzed desulfonative borylation of benzyl sulfones	5．発行年 2019年
3．雑誌名 Organic & Biomolecular Chemistry	6．最初と最後の頁 7300～7303
掲載論文のDOI（デジタルオブジェクト識別子） 10.1039/C9OB01099H	査読の有無 有
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1．著者名 Mina R. Narouz, Hannu Hakkinen, Tatsuya Tsukuda, Cathleen M. Crudden, et al	4．巻 印刷中
2．論文標題 N-heterocyclic carbene-functionalized magic-number gold nanoclusters	5．発行年 2019年
3．雑誌名 Nature Chemistry	6．最初と最後の頁 印刷中
掲載論文のDOI（デジタルオブジェクト識別子） 10.1038/s41557-019-0246-5	査読の有無 有
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1．著者名 Masakazu Nambo　Yasuyo Tahara　Dr. Jacky C.‐H. Yim, Cathleen M. Crudden	4．巻 25
2．論文標題 Cu‐Catalyzed Desulfonylative Amination of Benzhydryl Sulfones	5．発行年 2019年
3．雑誌名 Chemistry A European Journal	6．最初と最後の頁 1923-1926
掲載論文のDOI（デジタルオブジェクト識別子） 10.1002/chem.201805638	査読の有無 有
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2．論文標題 Generation and conversion of an N-heterocyclic carbene on Pt(111)	5．発行年 2018年
3．雑誌名 Chemical Communications	6．最初と最後の頁 12527-12530
掲載論文のDOI（デジタルオブジェクト識別子） 10.1039/C8CC06894A	査読の有無 有
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1．著者名 Zhijun Li, Kim Munro, Mina R. Narouz, Andrew Lau, Hongxia Hao, Cathleen M. Crudden, J. Hugh Horton	4．巻 10
2．論文標題 Self-Assembled N-Heterocyclic Carbene-Based Carboxymethylated Dextran Monolayers on Gold as a Tunable Platform for Designing Affinity-Capture Biosensor Surfaces	5．発行年 2018年
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掲載論文のDOI（デジタルオブジェクト識別子） 10.1021/acsami.8b02595	査読の有無 有
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2．論文標題 The Structural and Electrochemical Effects of N-Heterocyclic Carbene Monolayers on Magnesium	5．発行年 2018年
3．雑誌名 Journal of The Electrochemical Society	6．最初と最後の頁 G139-G145
掲載論文のDOI（デジタルオブジェクト識別子） 10.1149/2.0501811jes	査読の有無 有
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1．著者名 Larrea Christian R.、Baddeley Christopher J.、Narouz Mina R.、Mosey Nicholas J.、Horton J. Hugh、Crudden Cathleen M.	4．巻 18
2．論文標題 N-Heterocyclic Carbene Self-assembled Monolayers on Copper and Gold: Dramatic Effect of Wingtip Groups on Binding, Orientation and Assembly	5．発行年 2017年
3．雑誌名 ChemPhysChem	6．最初と最後の頁 3536～3539
掲載論文のDOI（デジタルオブジェクト識別子） 10.1002/cphc.201701045	査読の有無 有
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1．著者名 Man Renee W. Y.、Li Chien-Hung、MacLean Michael W. A.、Zenkina Olena V.、Zamora Matthew T.、Saunders Lisa N.、Rousina-Webb Alexander、Nambo Masakazu、Crudden Cathleen M.	4．巻 140
2．論文標題 Ultrastable Gold Nanoparticles Modified by Bidentate N-Heterocyclic Carbene Ligands	5．発行年 2018年
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1．著者名 Ariki Zachary T.、Maekawa Yuuki、Nambo Masakazu、Crudden Cathleen M.	4．巻 140
2．論文標題 Preparation of Quaternary Centers via Nickel-Catalyzed Suzuki?Miyaura Cross-Coupling of Tertiary Sulfones	5．発行年 2017年
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掲載論文のDOI（デジタルオブジェクト識別子） 10.1021/jacs.7b10855	査読の有無 有
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1．著者名 Clarke J. J.、Eisenberger P.、Piotrkowski S. S.、Crudden C. M.	4．巻 47
2．論文標題 Azaborines: synthesis and use in the generation of stabilized boron-substituted carbocations	5．発行年 2018年
3．雑誌名 Dalton Transactions	6．最初と最後の頁 1791～1795
掲載論文のDOI（デジタルオブジェクト識別子） 10.1039/C7DT01329A	査読の有無 有
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1．著者名 Rygus Jason P. G.、Crudden Cathleen M.	4．巻 139
2．論文標題 Enantiospecific and Iterative Suzuki-Miyaura Cross-Couplings	5．発行年 2017年
3．雑誌名 Journal of the American Chemical Society	6．最初と最後の頁 18124～18137
掲載論文のDOI（デジタルオブジェクト識別子） 10.1021/jacs.7b08326	査読の有無 有
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1．著者名 Narouz Mina R.、Li Chien-Hung、Nazemi Ali、Crudden Cathleen M.	4．巻 33
2．論文標題 Amphiphilic N-Heterocyclic Carbene-Stabilized Gold Nanoparticles and Their Self-Assembly in Polar Solvents	5．発行年 2017年
3．雑誌名 Langmuir	6．最初と最後の頁 14211～14219
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1．著者名 Li Zhijun、Munro Kim、Ebralize Iraklli I.、Narouz Mina R.、Padmos J. Daniel、Hao Hongxia、Crudden Cathleen M.、Horton J. Hugh	4．巻 33
2．論文標題 N-Heterocyclic Carbene Self-Assembled Monolayers on Gold as Surface Plasmon Resonance Biosensors	5．発行年 2017年
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3．雑誌名 ACS Applied Materials & Interfaces	6．最初と最後の頁 39223～39234
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1．著者名 Nambo Masakazu、Crudden Cathleen、Yim Jacky、Fowler Kevin	4．巻 28
2．論文標題 Synthesis of Tetraarylmethanes by the Triflic Acid-Promoted Formal Cross-Dehydrogenative Coupling of Triarylmethanes with Arenes	5．発行年 2017年
3．雑誌名 Synlett	6．最初と最後の頁 2936～2940
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1．著者名 Yim Jacky C.-H.、Nambo Masakazu、Crudden Cathleen M.	4．巻 19
2．論文標題 Pd-Catalyzed Desulfonative Cross-Coupling of Benzylic Sulfone Derivatives with 1,3-Oxazoles	5．発行年 2017年
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〔学会発表〕　計20件（うち招待講演　11件／うち国際学会　8件）

1．発表者名
Cathleen Crudden

2．発表標題
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1．発表者名
Cathleen Crudden

2．発表標題
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4．発表年
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1．発表者名
Cathleen Crudden

2．発表標題
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1．発表者名
Cathleen Crudden

2．発表標題
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１．発表者名
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１．発表者名
Cathleen Crudden

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Cathleen Crudden

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１．発表者名
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１．発表者名
Cathleen M. Crudden

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Impact of Research on Training of Highly Qualified Personnel (HQP)

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１．発表者名
Cathleen M. Crudden

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３．学会等名
Southern Ontario Undergraduate Student Chemistry Conference

４．発表年
2018年

〔図書〕　計0件

〔産業財産権〕

〔その他〕

IPMI Carol Tyler Award
https://www.ipmi.org
2017 Queen's Prize for Excellence in Research
http://www.chem.queensu.ca
Congratulations to SYNLETT Best Paper Award 2017
https://www.thieme.de/en/thieme-chemistry/2017-winners-123200.htm
SYNLETT Best Paper Award 2017
http://www.itbm.nagoya-u.ac.jp/en/news/2018/02/Crudden-Synlett.php

６．研究組織

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