

Supporting information

Orbital Control of Single-Molecule Conductance Perturbed by p-accepting Anchor Groups: Cyanide and Isocyanide

Junya Koga, Yuta Tsuji, and Kazunari Yoshizawa*

Institute for Materials Chemistry and Engineering and International Research Center for Molecular Systems, Kyushu University, Fukuoka 819-0395, Japan

*To whom correspondence should be addressed.

E-mail: kazunari@ms.ifoc.kyushu-u.ac.jp

Table of contents

Reference 63	2
Table S1.	3
Table S2.	6
Table S3.	9
Table S4.	12

Reference

(63) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., Gaussian 09, Revision A.01; Gaussian, Inc., Wallingford CT, 2009.

Table S1. Geometrical parameters of the central regions with *p*-BDCN. Units are in Å.

atom	x	y	z
Au	-3.605235000	7.074898000	1.177289000
Au	2.162282000	7.074898000	1.177289000
Au	-0.721476300	7.074898000	1.177289000
Au	3.604161000	4.577490000	1.177289000
Au	-2.163355000	4.577490000	1.177289000
Au	0.720402800	4.577490000	1.177289000
Au	-0.721476300	2.080082000	1.177289000
Au	2.162282000	2.080082000	1.177289000
Au	5.046040000	2.080082000	1.177289000
Au	0.720402800	2.912551000	3.531868000
Au	-0.721476300	5.409959000	3.531868000
Au	5.046040000	5.409959000	3.531868000
Au	3.604161000	2.912551000	3.531868000
Au	2.162282000	5.409959000	3.531868000
Au	6.487919000	2.912551000	3.531868000
Au	5.046040000	0.415143300	3.531868000
Au	2.162282000	0.415143300	3.531868000
Au	7.929798000	0.415143300	3.531868000
Au	3.604161000	6.242428000	5.886447000
Au	5.046040000	3.745021000	5.886447000
Au	0.720402800	1.247613000	5.886447000
Au	-0.721476300	3.745021000	5.886447000
Au	0.720402800	6.242428000	5.886447000
Au	2.162282000	3.745021000	5.886447000
Au	3.604161000	1.247613000	5.886447000
Au	-2.163355000	6.242428000	5.886447000
Au	6.487919000	1.247613000	5.886447000
N	2.162130000	3.744245000	8.115006000
C	2.162619000	3.744360000	9.285241000

C	2.162885000	3.744965000	10.688600000
H	2.146578000	5.914887000	10.828690000
H	2.179692000	1.574925000	10.832380000
C	2.153515000	4.968598000	11.390390000
C	2.172322000	2.522356000	11.392200000
C	2.153252000	4.969770000	12.766700000
C	2.172100000	2.523514000	12.768540000
H	2.145983000	5.917256000	13.326420000
H	2.179292000	1.577155000	13.330130000
C	2.162413000	3.747170000	13.470340000
C	2.162051000	3.748203000	14.873680000
N	2.161714000	3.749023000	16.043960000
Au	-2.163751000	6.245988000	18.272900000
Au	6.487524000	1.251172000	18.272900000
Au	5.045645000	3.748580000	18.272900000
Au	0.720007400	1.251172000	18.272900000
Au	3.603766000	6.245988000	18.272900000
Au	0.720007400	6.245988000	18.272900000
Au	3.603766000	1.251172000	18.272900000
Au	-0.721871800	3.748580000	18.272900000
Au	2.161886000	3.748580000	18.272900000
Au	3.603766000	4.581049000	20.627480000
Au	2.161886000	7.078457000	20.627480000
Au	-0.721871800	2.083641000	20.627480000
Au	5.045645000	2.083641000	20.627480000
Au	-0.721871800	7.078457000	20.627480000
Au	0.720007400	4.581049000	20.627480000
Au	2.161886000	2.083641000	20.627480000
Au	-3.605630000	7.078457000	20.627480000
Au	-2.163751000	4.581049000	20.627480000
Au	6.487524000	2.916110000	22.982060000
Au	5.045645000	5.413518000	22.982060000

Au	2.161886000	0.418702600	22.982060000
Au	2.161886000	5.413518000	22.982060000
Au	3.603766000	2.916110000	22.982060000
Au	-0.721871800	5.413518000	22.982060000
Au	0.720007400	2.916110000	22.982060000
Au	5.045645000	0.418702600	22.982060000
Au	7.929403000	0.418702600	22.982060000

Table S2. Geometrical parameters of the central regions with *p*-BDNC. Units are in Å.

atom	x	y	z
Au	-3.605761000	7.077180000	1.177289000
Au	2.161755000	7.077180000	1.177289000
Au	-0.722002900	7.077180000	1.177289000
Au	-2.163882000	4.579772000	1.177289000
Au	3.603634000	4.579772000	1.177289000
Au	0.719876200	4.579772000	1.177289000
Au	-0.722002900	2.082364000	1.177289000
Au	5.045514000	2.082364000	1.177289000
Au	2.161755000	2.082364000	1.177289000
Au	5.045514000	5.412242000	3.531868000
Au	-0.722002900	5.412242000	3.531868000
Au	2.161755000	5.412242000	3.531868000
Au	0.719876200	2.914834000	3.531868000
Au	3.603634000	2.914834000	3.531868000
Au	6.487393000	2.914834000	3.531868000
Au	7.929272000	0.417425800	3.531868000
Au	5.045514000	0.417425800	3.531868000
Au	2.161755000	0.417425800	3.531868000
Au	3.603634000	6.244711000	5.886447000
Au	5.045514000	3.747303000	5.886447000
Au	2.161755000	3.747303000	5.886447000
Au	0.719876200	6.244711000	5.886447000
Au	-2.163882000	6.244711000	5.886447000
Au	-0.722002900	3.747303000	5.886447000
Au	3.603634000	1.249895000	5.886447000
Au	0.719876200	1.249895000	5.886447000
Au	6.487393000	1.249895000	5.886447000
C	2.161652000	3.745976000	7.900336000
N	2.161856000	3.747125000	9.083744000

C	2.162230000	3.746762000	10.428400000
H	2.195806000	1.584892000	10.549880000
H	2.128727000	5.908528000	10.551560000
C	2.181505000	2.524630000	11.122250000
C	2.143418000	4.968348000	11.123190000
C	2.181991000	2.524104000	12.499850000
C	2.143901000	4.967836000	12.500810000
H	2.196678000	1.583823000	13.071310000
H	2.129585000	5.907690000	13.072990000
C	2.163176000	3.745693000	13.194730000
N	2.163521000	3.745187000	14.539420000
C	2.163613000	3.745476000	15.722890000
Au	-2.162134000	6.241358000	17.736980000
Au	5.047262000	3.743950000	17.736980000
Au	6.489141000	1.246542000	17.736980000
Au	0.721624700	1.246542000	17.736980000
Au	3.605383000	6.241358000	17.736980000
Au	0.721624700	6.241358000	17.736980000
Au	3.605383000	1.246542000	17.736980000
Au	-0.720254400	3.743950000	17.736980000
Au	2.163504000	3.743950000	17.736980000
Au	3.605383000	4.576419000	20.091550000
Au	2.163504000	7.073827000	20.091550000
Au	0.721624700	4.576419000	20.091550000
Au	5.047262000	2.079011000	20.091550000
Au	-0.720254400	7.073827000	20.091550000
Au	2.163504000	2.079011000	20.091550000
Au	-3.604013000	7.073827000	20.091550000
Au	-2.162134000	4.576419000	20.091550000
Au	-0.720254400	2.079011000	20.091550000
Au	5.047262000	5.408888000	22.446130000
Au	6.489141000	2.911481000	22.446130000

Au	2.163504000	0.414072700	22.446130000
Au	2.163504000	5.408888000	22.446130000
Au	3.605383000	2.911481000	22.446130000
Au	-0.720254400	5.408888000	22.446130000
Au	0.721624700	2.911481000	22.446130000
Au	5.047262000	0.414072700	22.446130000
Au	7.931020000	0.414072700	22.446130000

Table S3. Geometrical parameters of the central regions with *m*-BDCN. Units are in Å.

atom	x	y	z
Au	0.720939600	6.588604000	1.177289000
Au	3.604698000	6.588604000	1.177289000
Au	-2.162819000	6.588604000	1.177289000
Au	5.046577000	4.091196000	1.177289000
Au	-0.720939600	4.091196000	1.177289000
Au	2.162819000	4.091196000	1.177289000
Au	0.720939600	1.593788000	1.177289000
Au	6.488456000	1.593788000	1.177289000
Au	3.604698000	1.593788000	1.177289000
Au	-0.720939600	7.421073000	3.531868000
Au	-2.162819000	4.923666000	3.531868000
Au	0.720939600	4.923666000	3.531868000
Au	3.604698000	4.923666000	3.531868000
Au	-3.604698000	7.421073000	3.531868000
Au	2.162819000	7.421073000	3.531868000
Au	5.046577000	2.426258000	3.531868000
Au	2.162819000	2.426258000	3.531868000
Au	-0.720939600	2.426258000	3.531868000
Au	6.488456000	3.258727000	5.886447000
Au	5.046577000	5.756135000	5.886447000
Au	2.162819000	5.756135000	5.886447000
Au	3.604698000	3.258727000	5.886447000
Au	-0.720939600	5.756135000	5.886447000
Au	0.720939600	3.258727000	5.886447000
Au	2.162819000	0.761319000	5.886447000
Au	7.930335000	0.761319000	5.886447000
Au	5.046577000	0.761319000	5.886447000
N	2.162819000	5.756135000	8.115007000
C	2.162819000	5.174761000	9.121976000

H	2.162819000	2.516854000	9.405283000
C	2.162819000	3.045351000	10.352840000
C	2.162819000	4.450824000	10.361000000
H	2.162819000	1.259204000	11.549490000
C	2.162819000	2.344608000	11.556830000
C	2.162819000	5.148877000	11.575810000
H	2.162819000	6.233020000	11.583150000
C	2.162819000	3.028989000	12.770200000
C	2.162819000	4.434444000	12.781070000
H	2.162819000	2.487713000	13.710520000
C	2.162819000	5.141533000	14.029770000
N	2.162819000	5.709220000	15.044580000
Au	3.604698000	3.211812000	17.273140000
Au	6.488456000	3.211812000	17.273140000
Au	-0.720939600	5.709220000	17.273140000
Au	0.720939600	3.211812000	17.273140000
Au	5.046577000	5.709220000	17.273140000
Au	2.162819000	5.709220000	17.273140000
Au	2.162819000	0.714404100	17.273140000
Au	7.930335000	0.714404100	17.273140000
Au	5.046577000	0.714404100	17.273140000
Au	-0.720939600	4.044281000	19.627720000
Au	-2.162819000	6.541689000	19.627720000
Au	3.604698000	6.541689000	19.627720000
Au	6.488456000	1.546873000	19.627720000
Au	3.604698000	1.546873000	19.627720000
Au	5.046577000	4.044281000	19.627720000
Au	0.720939600	6.541689000	19.627720000
Au	2.162819000	4.044281000	19.627720000
Au	0.720939600	1.546873000	19.627720000
Au	2.162819000	7.374158000	21.982300000
Au	2.162819000	2.379343000	21.982300000

Au	5.046577000	2.379343000	21.982300000
Au	-0.720939600	7.374158000	21.982300000
Au	-2.162819000	4.876751000	21.982300000
Au	0.720939600	4.876751000	21.982300000
Au	-3.604698000	7.374158000	21.982300000
Au	3.604698000	4.876751000	21.982300000
Au	-0.720939600	2.379343000	21.982300000

Table S4. Geometrical parameters of the central regions with *m*-BDNC. Units are in Å.

atom	x	y	z
Au	0.720939600	6.566144000	1.177289000
Au	-2.162819000	6.566144000	1.177289000
Au	3.604698000	6.566144000	1.177289000
Au	5.046577000	4.068736000	1.177289000
Au	-0.720939600	4.068736000	1.177289000
Au	2.162819000	4.068736000	1.177289000
Au	0.720939600	1.571328000	1.177289000
Au	6.488456000	1.571328000	1.177289000
Au	3.604698000	1.571328000	1.177289000
Au	-3.604698000	7.398613000	3.531868000
Au	0.720939600	4.901205000	3.531868000
Au	3.604698000	4.901205000	3.531868000
Au	-2.162819000	4.901205000	3.531868000
Au	2.162819000	7.398613000	3.531868000
Au	-0.720939600	7.398613000	3.531868000
Au	5.046577000	2.403797000	3.531868000
Au	2.162819000	2.403797000	3.531868000
Au	-0.720939600	2.403797000	3.531868000
Au	5.046577000	5.733674000	5.886447000
Au	7.930335000	0.738858700	5.886447000
Au	2.162819000	5.733674000	5.886447000
Au	5.046577000	0.738858700	5.886447000
Au	3.604698000	3.236267000	5.886447000
Au	2.162819000	0.738858700	5.886447000
Au	-0.720939600	5.733674000	5.886447000
Au	0.720939600	3.236267000	5.886447000
Au	6.488456000	3.236267000	5.886447000
C	2.162819000	5.733674000	7.900337000
N	2.162819000	5.142699000	8.923936000

H	2.162819000	2.519965000	9.151447000
C	2.162819000	3.041843000	10.102030000
C	2.162819000	4.443232000	10.117500000
H	2.162819000	1.260908000	11.303140000
C	2.162819000	2.346387000	11.309250000
C	2.162819000	5.147887000	11.325070000
H	2.162819000	6.231316000	11.331150000
C	2.162819000	3.028208000	12.524230000
C	2.162819000	4.429695000	12.524640000
H	2.162819000	2.495626000	13.468860000
N	2.162819000	5.115651000	13.726010000
C	2.162819000	5.695193000	14.756110000
Au	5.046577000	0.700377200	16.770000000
Au	3.604698000	3.197785000	16.770000000
Au	2.162819000	0.700377200	16.770000000
Au	6.488456000	3.197785000	16.770000000
Au	0.720939600	3.197785000	16.770000000
Au	-0.720939600	5.695193000	16.770000000
Au	5.046577000	5.695193000	16.770000000
Au	7.930335000	0.700377200	16.770000000
Au	2.162819000	5.695193000	16.770000000
Au	-2.162819000	6.527662000	19.124580000
Au	6.488456000	1.532847000	19.124580000
Au	3.604698000	6.527662000	19.124580000
Au	-0.720939600	4.030254000	19.124580000
Au	3.604698000	1.532847000	19.124580000
Au	5.046577000	4.030254000	19.124580000
Au	0.720939600	6.527662000	19.124580000
Au	2.162819000	4.030254000	19.124580000
Au	0.720939600	1.532847000	19.124580000
Au	2.162819000	7.360132000	21.479160000
Au	2.162819000	2.365316000	21.479160000

Au	5.046577000	2.365316000	21.479160000
Au	-0.720939600	7.360132000	21.479160000
Au	-2.162819000	4.862724000	21.479160000
Au	0.720939600	4.862724000	21.479160000
Au	-3.604698000	7.360132000	21.479160000
Au	3.604698000	4.862724000	21.479160000
Au	-0.720939600	2.365316000	21.479160000