Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Materials

Photoelectron Spectroscopy and Density Functional Study of $Co_nC_2^-$ (n=1-5) Clusters

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Contents:

1. Cartesian Coordinates of $Co_nC_2^-$ (n=1-5) clusters anions in the article.

1A

C	0.00000000	0.66436200	-1.20244300
C	0.00000000	-0.66436200	-1.20244300
Co	0.00000000	0.00000000	0.53441900

1B

C	0.00000000	0.00000000	-1.03018000
C	0.00000000	0.00000000	-2.31480500
Co	0.00000000	0.00000000	0.74333000

1C

C	0.00000000	0.65799000	-1.24550600
C	0.00000000	-0.65799000	-1.24550600
Co	0.00000000	0.00000000	0.55355800

2A

C	1.17288500	-0.57397600	0.00000000
C	1.82482400	0.56352800	0.00000000
Co	-0.66615800	-1.04307100	0.00000000
Co	0.00000000	1.04539300	0.00000000

2B

C	1.03129000	-0.51323300	0.00000000
C	1.82092300	0.54618500	0.00000000
Co	-0.63382500	-1.11976000	0.00000000
Co	0.00000000	1.11243700	0.00000000

2C

C	0.00000000	0.63674700	0.00011400
C	0.00000000	-0.63674700	0.00011400
Co	0.00000000	2.39712400	-0.00002500
Co	0.00000000	-2.39712400	-0.00002500

3A

Co	-0.63821100	-0.95434200	-0.13200600
Co	1.54420700	-0.36233000	0.10362500
Co	0.02343100	1.23792600	-0.08712600
C	-1.73632900	0.72313300	0.25559200
C	-2.44609600	-0.36877300	0.26418400

3B

C	-0.04247300	1.09656800	0.66812100

C	-0.04247300	1.09656800	-0.66812100
Co	-0.04247300	0.11863700	-2.17772500
Co	0.10382400	-0.72463700	0.00000000
Co	-0.04247300	0.11863700	2.17772500

3C

C	0.07843600	1.03888600	0.66350300
C	0.07843600	1.03888600	-0.66350300
Co	0.07843600	0.15542100	-2.17720200
Co	-0.19173200	-0.77257000	0.00000000
Co	0.07843600	0.15542100	2.17720200

3D

C	-1.31891100	-0.00127500	1.14967000
C	0.03305000	-0.00074200	1.25881700
Co	1.44542900	0.00037500	0.00857700
Co	-0.58022400	1.13204400	-0.27165500
Co	-0.57945700	-1.13197100	-0.27214100

4A

C	-2.13499400	0.01984900	-0.17880000
C	-1.24313900	0.97507000	-0.49136600
Co	0.58774300	1.26800200	-0.42344200
Co	-0.50376400	-0.87090000	-0.93705200
Co	-0.72652300	0.02071400	1.20142400
Co	1.39324100	-0.63890900	0.30799500

4B

Co	0.89243300	-0.79945700	-0.55633800
Co	-1.36115700	0.45856500	-0.72345900
Co	-0.82027700	-1.04455800	0.76430600
Co	0.23923300	1.27924500	0.49378900
C	2.03278700	0.75893300	0.25862600
C	2.69116400	-0.28101400	-0.16096600

4C

Co	0.08375200	-0.78013600	-1.15663000
C	-2.38767200	0.12318100	0.00798200
Co	0.10514300	-0.76907300	1.16178100
Co	-0.79382000	1.12570100	0.00015600
C	-1.44066600	-0.82116300	0.01649600
Co	1.45566700	0.57861500	-0.01074700

4D

Co	0.82659600	-0.97283000	-0.00041900
Co	-1.04437600	-0.20661800	-1.11575600
Co	-1.04328500	-0.20680100	1.11635400
Co	0.23187000	1.32102800	-0.00009800
C	1.97513000	0.70660700	0.00005800
C	2.65625500	-0.41311200	-0.00042300

4E

Co	-1.19701500	-0.51745200	0.00000000
C	0.36630900	-1.58366200	0.66642900
Co	0.36630900	-0.05012300	-1.71781400
Co	0.36630900	-0.05012300	1.71781400
C	0.36630900	-1.58366200	-0.66642900
Co	0.30159300	1.32154700	0.00000000

4F

Co	-0.24448800	-0.77148600	1.13960000
C	-1.86480800	-1.02192900	0.00000000
Co	-0.24448800	1.53582500	0.00000000
Co	-0.24448800	-0.77148600	-1.13960000
C	-1.66025500	0.29947000	0.00000000
Co	1.51681100	0.16769400	0.00000000

4G

Co	0.08110800	-1.03233900	0.29152500
Co	2.07406900	-0.30639400	-0.30875300
Co	-1.63122300	0.61079600	-0.24617000
C	-2.89441000	-0.83454100	-0.14512300
C	-1.75361600	-1.41991100	0.05696000
Co	0.50894000	1.22892600	0.28298900

4H

Co	0.23943200	-0.67407800	1.22625300
C	2.11762800	1.15440800	0.00000000
Co	0.23943200	-0.67407800	-1.22625300
Co	0.23943200	1.38906700	0.00000000
C	1.63877500	-0.08165600	0.00000000
Co	-1.55305300	-0.27930000	0.00000000

5A

Co	-0.09652500	-0.93878200	-0.88645900
Co	0.48199400	1.38126100	-0.32508100
Co	0.12611000	-0.16800100	1.35050300
C	-2.08513800	-1.31361800	-0.31131800

C	-1.35006300	-1.19388800	0.78074300
Co	1.94384700	-0.33654400	-0.11574900
Co	-1.69204800	0.61928900	-0.12753100

5B

Co	-1.94551200	-0.33414700	-0.11322200
Co	-0.12274500	-0.16234100	1.35320200
Co	-0.47935800	1.37804300	-0.33005000
Co	1.69415200	0.61632200	-0.12884900
Co	0.09115500	-0.93937800	-0.88353400
C	2.08321500	-1.31785900	-0.31535500
C	1.34717000	-1.19538800	0.77639500

5C

Co	0.00063000	-0.34896800	0.84423700
Co	-1.21871300	1.35114100	-0.09491200
Co	1.97307800	-0.72110300	-0.28928100
C	0.66114300	-2.04258800	-0.15104700
C	-0.65484300	-2.04559500	-0.15146600
Co	1.21308500	1.35355200	-0.10021000
Co	-1.96947900	-0.72613800	-0.29260900

5D

Co	-2.00688600	-0.26766300	-0.07710400
Co	-0.15109700	-0.14068000	1.35248200
Co	-0.45979200	1.28390400	-0.40944400
Co	1.79568200	0.56902000	-0.05115300
Co	0.10128600	-0.89807400	-0.89777000
C	1.97778100	-1.30916100	-0.38499400
C	1.26585200	-1.15012200	0.75844600

5E

Co	-0.09999000	-0.89903900	-0.89623000
Co	0.46039400	1.28335300	-0.40970200
Co	0.14916500	-0.13928400	1.35277900
C	-1.97744400	-1.31012500	-0.38487800
C	-1.26667400	-1.14899400	0.75898600
Co	2.00698900	-0.26766200	-0.07670100
Co	-1.79564400	0.56910300	-0.05328200

5F

Co	-0.23819600	0.34477200	1.09666400
Co	1.84143000	-0.68263100	0.47167900
Co	-2.12544400	-0.43375400	-0.04357700

C	-1.71380200	1.31715000	0.02440400
C	-0.53608800	1.87227400	-0.24431400
Co	-0.02835800	-0.99718700	-0.76996800
Co	1.05054400	1.06004000	-0.70592900

5G

Co	-0.40736600	1.12165300	-0.00324200
Co	-2.41827700	0.16188900	0.00675700
Co	1.26250800	-0.26053000	-1.14895600
C	2.58680600	0.66961600	0.03692400
C	1.49060800	1.42686400	0.03035500
Co	-0.57238000	-1.19338800	-0.02467300
Co	1.22942300	-0.29550700	1.15516200

2. Cartesian Coordinates of Co_nC_2 (n=1-5) clusters neutrals in the article.

CoC_2

C	0.00000000	0.66850800	-1.18509700
C	0.00000000	-0.66850800	-1.18509700
Co	0.00000000	0.00000000	0.52671000

Co_2C_2

C	1.04857200	-0.53015600	0.00000000
C	1.78982600	0.55777800	0.00000000
Co	-0.63075500	-1.11388000	0.00000000
Co	0.00000000	1.10774200	0.00000000

Co_3C_2

Co	-1.30340600	0.66721700	0.00000000
Co	0.42179900	-0.51534400	1.14306900
Co	0.42179900	-0.51534400	-1.14306900
C	1.64733800	0.53578300	0.00000000
C	0.42179900	1.09983500	0.00000000

Co_4C_2

C	-2.09183200	0.16845400	-0.01451100
C	-1.20172900	1.15971600	-0.02045000
Co	0.65148100	1.33306900	-0.01492500
Co	-0.62545700	-0.44954400	-1.17134100
Co	-0.63972600	-0.41524600	1.17955400
Co	1.34560400	-0.76342900	0.01448000

Co_5C_2

Co	-0.13311200	-0.80210300	-1.04289400

Co	0.47361100	1.30042900	-0.35035100
Co	0.16002900	-0.28789800	1.32377700
C	-1.89076000	-1.30211500	-0.50005900
C	-1.33379400	-1.19321000	0.71663100
Co	1.99545600	-0.25566200	-0.03826900
Co	-1.77941600	0.59975100	0.05961000