Ca-Ca interaction in inverse sandwich Ca-C_8H_8-Ca

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1. The detailed Cartesian coordinates of Ca-C_8H_8-Ca obtained at PBEPBE/def2-TZVPP level.

close-shell singlet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 1

C	-0.00028900	0.30295300	-1.83077700
C	-0.00052700	1.50901200	-1.08016200
C	-0.00080000	1.83079600	0.30295400
C	0.00046600	-1.08016600	-1.50900000
C	-0.00044800	1.08016700	1.50900000
C	0.00082000	-1.83079500	-0.30295400
C	0.00054500	-1.50901100	1.08016200
H	-0.00051500	0.48086100	-2.90617600
H	-0.00061000	2.39525300	-1.71471600
H	-0.00125900	2.90619500	0.48086000
H	0.00067500	-1.71470400	-2.39525400
H	0.00127300	-2.90619400	-0.48086000
C	0.00030800	-0.30295200	1.83077800
H	-0.00065600	1.71470400	2.39525400
H	0.00052900	-0.48086000	2.90617700
H	0.00062900	-2.39525200	1.71471600
Ca	-1.97519600	-0.00060300	0.00003800
Ca	1.97517000	0.00060200	-0.00003900

State=1-A\HF=-1664.108278\S2=0.\S2-1=0.\S2A=0

open-shell singlet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 1

C	-0.00028900	0.31317300	-1.82905600
C	-0.00052800	1.51502100	-1.07171700
C	-0.00080100	1.82907500	0.31317500
C	0.00046700	-1.07172100	-1.51500900
C	-0.00044900	1.07172200	1.51501000
C	0.00082100	-1.82907400	-0.31317400
C	0.00054600	-1.51502000	1.07171700
H	-0.00051500	0.49708500	-2.90344500
H	-0.00061100	2.40479300	-1.70131100
H	-0.00126000	2.90346400	0.49708400

H	0.00067600	-1.70129900	-2.40479300
H	0.00127400	-2.90346300	-0.49708400
C	0.00030800	-0.31317300	1.82905800
H	-0.00065700	1.70129900	2.40479400
H	0.00052900	-0.49708400	2.90344600
H	0.00063000	-2.40479200	1.70131200
Ca	-1.97519600	-0.00060400	0.00003500
Ca	1.97517000	0.00060300	-0.00003500

State=1-A\HF=-1664.1129903\S2=0.706695\S2-1=0.\S2A=0.00205

triplet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 3

C	-0.00012700	-0.73909400	1.70132500
C	-0.00033500	-1.72591900	0.68044400
C	-0.00048700	-1.70133500	-0.73909400
C	0.00029200	0.68044500	1.72590700
C	-0.00028600	-0.68044400	-1.72590600
C	0.00049100	1.70133600	0.73909400
C	0.00034000	1.72592000	-0.68044300
H	-0.00025600	-1.17344600	2.70122500
H	-0.00036300	-2.74015100	1.08011200
H	-0.00076900	-2.70123100	-1.17345300
H	0.00041900	1.08010500	2.74014300
H	0.00076300	2.70123200	1.17345400
C	0.00013000	0.73909500	-1.70132400
H	-0.00041600	-1.08010400	-2.74014300
H	0.00025000	1.17344700	-2.70122400
H	0.00036600	2.74015200	-1.08011200
Ca	-1.98352000	0.00035400	0.00008600
Ca	1.98351500	-0.00035500	-0.00008700

State=3-A\HF=-1664.1080058\S2=2.00053\S2-1=0.\S2A=2

2. The detailed Cartesian coordinates of Ca-C_8H_8-Ca obtained at BP86/def2-TZVPP level.

close-shell singlet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 1

C	0.00009800	-0.02707500	1.85732300
C	0.00022100	-1.33251300	1.29417200
C	0.00036500	-1.85732500	-0.02707500
C	-0.00023700	1.29417300	1.33251200
C	0.00023700	-1.29417200	-1.33251200
C	-0.00036400	1.85732600	0.02707500
C	-0.00022200	1.33251400	-1.29417200
H	0.00018000	-0.04307800	2.94748300
H	0.00024200	-2.11466300	2.05371200
H	0.00057200	-2.94748600	-0.04307800
H	-0.00035900	2.05371200	2.11466400
H	-0.00057900	2.94748700	0.04307800
C	-0.00009800	0.02707500	-1.85732200
H	0.00035600	-2.05371100	-2.11466400
H	-0.00018800	0.04307900	-2.94748300
H	-0.00024500	2.11466300	-2.05371200
Ca	-1.98002600	-0.00026900	0.00002800
Ca	1.98002700	0.00026800	-0.00002800

State=1-A\HF=-1665.0905949

open-shell singlet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 1

C	0.00007600	-1.84716600	0.19487100
C	0.00008100	-1.16807900	1.44352000
C	0.00014600	0.19487100	1.84716500
C	-0.00007700	-1.44352100	-1.16807900
C	0.00007700	1.44352100	1.16807900
C	-0.00014500	-0.19487100	-1.84716500
C	-0.00008200	1.16807900	-1.44352000
H	0.00013500	-2.93173800	0.30913400
H	0.00006800	-1.85434700	2.29121700
H	0.00022900	0.30913400	2.93173600
H	-0.00010700	-2.29121700	-1.85434700
H	-0.00023100	-0.30913500	-2.93173500
C	-0.00007700	1.84716700	-0.19487200
H	0.00010700	2.29121700	1.85434700
H	-0.00013800	2.93173800	-0.30913400
H	-0.00006900	1.85434700	-2.29121800
Ca	1.98684300	0.00002000	-0.00010100
Ca	-1.98684300	-0.00002000	0.00010100

State=1-A\HF=-1665.0955515\S2=0.744329\S2-1=0.\S2A=0.004126

triplet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 3

C	0.00006300	0.30158300	-1.83213600
C	0.00015200	1.50877500	-1.08218500
C	0.00021300	1.83213900	0.30158200
C	-0.00012600	-1.08218500	-1.50877300
C	0.00012600	1.08218700	1.50877300
C	-0.00021300	-1.83213700	-0.30158200
C	-0.00015200	-1.50877400	1.08218600
H	0.00011900	0.47876900	-2.90823500
H	0.00016500	2.39486900	-1.71796000
H	0.00033200	2.90823700	0.47876900
H	-0.00019200	-1.71795900	-2.39486800
H	-0.00033900	-2.90823600	-0.47876900
C	-0.00006400	-0.30158100	1.83213600
H	0.00019000	1.71796000	2.39486800
H	-0.00012600	-0.47876800	2.90823500
H	-0.00016700	-2.39486800	1.71796000
Ca	-1.99421000	0.00016000	-0.00000500
Ca	1.99421100	-0.00016100	0.00000400

State=3-A\HF=-1665.0909366\S2=2.001017\S2-1=0.\S2A=2.000001

3. The detailed Cartesian coordinates of Ca-C_8H_8-Ca obtained at X3LYP/def2-TZVPP level.

close-shell singlet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 1

C	-0.00005300	1.81151400	-0.35604700
C	-0.00008600	1.02918700	-1.53269100
C	-0.00012400	-0.35604700	-1.81151000
C	0.00005900	1.53269300	1.02918600
C	-0.00006800	-1.53269300	-1.02918600
C	0.00011500	0.35604700	1.81151000
C	0.00007600	-1.02918600	1.53269100
H	-0.00009700	2.87205400	-0.56440100
H	-0.00007900	1.63159100	-2.43004700
H	-0.00019200	-0.56440000	-2.87205100
H	0.00008500	2.43004700	1.63159300
H	0.00018100	0.56440000	2.87205000
C	0.00004400	-1.81151400	0.35604700
H	-0.00009400	-2.43004700	-1.63159300
H	0.00008600	-2.87205400	0.56440100
H	0.00007000	-1.63159100	2.43004700
Ca	2.00742000	0.00000600	-0.00008600
Ca	-2.00740700	-0.00000600	0.00008600

State=1-A\HF=-1664.7182855

open-shell singlet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 1

C	-0.00003800	-1.72472600	0.65653000
C	-0.00008700	-0.75523900	1.68373400
C	-0.00012600	0.65653000	1.72472100
C	0.00007200	-1.68373800	-0.75523900
C	-0.00007200	1.68373700	0.75523900
C	0.00012500	-0.65653000	-1.72472100
C	0.00008700	0.75524000	-1.68373400
H	-0.00007500	-2.73517700	1.04115800
H	-0.00008700	-1.19753100	2.67028700
H	-0.00019300	1.04115500	2.73517500
H	0.00009900	-2.67028900	-1.19753300
H	0.00019000	-1.04115600	-2.73517500
C	0.00003800	1.72472500	-0.65653000
H	-0.00009900	2.67029000	1.19753300
H	0.00007100	2.73517700	-1.04115800
H	0.00008600	1.19753100	-2.67028700
Ca	2.02303300	0.00001500	0.00008900
Ca	-2.02303200	-0.00001500	-0.00008900

State=1-A\HF=-1664.7264286\S2=0.841905\S2-1=0.\S2A=0.00098

triplet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 3

C	-0.00003900	-1.68916100	0.74326600
C	-0.00008700	-0.66876300	1.71991300
C	-0.00012500	0.74326600	1.68915700
C	0.00007100	-1.71991700	-0.66876300
C	-0.00007100	1.71991700	0.66876300
C	0.00012500	-0.74326600	-1.68915700
C	0.00008700	0.66876400	-1.71991300
H	-0.00007600	-2.67877700	1.17871000
H	-0.00008700	-1.06038600	2.72765400
H	-0.00019200	1.17870700	2.67877500
H	0.00009700	-2.72765600	-1.06038800
H	0.00018900	-1.17870700	-2.67877500
C	0.00003900	1.68916100	-0.74326600
H	-0.00009700	2.72765700	1.06038800
H	0.00007300	2.67877700	-1.17871000
H	0.00008700	1.06038600	-2.72765400
Ca	2.02303300	0.00001800	0.00008800
Ca	-2.02303200	-0.00001800	-0.00008800

State=3-A\HF=-1664.7228444\S2=2.000149\S2-1=0.\S2A=2.

4. The detailed Cartesian coordinates of Ca-C_8H_8-Ca obtained at MP2/def2-TZVPP level.

close-shell singlet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 1

C	-0.00002500	1.83511900	-0.25609100
C	-0.00006300	1.11654100	-1.47870800
C	-0.00008000	-0.25609100	-1.83511700
C	0.00004500	1.47870900	1.11654000
C	-0.00004300	-1.47870900	-1.11654000
C	0.00008100	0.25609100	1.83511700
C	0.00006400	-1.11654100	1.47870800
H	-0.00004300	2.90671600	-0.40563400
H	-0.00008400	1.76853300	-2.34218300
H	-0.00012600	-0.40563300	-2.90671400
H	0.00006600	2.34218300	1.76853400
H	0.00012700	0.40563300	2.90671400
C	0.00002600	-1.83511800	0.25609100
H	-0.00006400	-2.34218300	-1.76853400
H	0.00004500	-2.90671600	0.40563400
H	0.00008600	-1.76853300	2.34218300
Ca	2.08530900	0.00000600	-0.00006000
Ca	-2.08531100	-0.00000700	0.00006000

State=1-A\MP2=-1662.5982418

open-shell singlet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 1

C	-0.00001000	0.14510900	-1.84692700
C	-0.00001900	1.40858200	-1.20336700
C	-0.00002600	1.84692800	0.14510900
C	0.00001400	-1.20336700	-1.40858200
C	-0.00001400	1.20336700	1.40858200
C	0.00002600	-1.84692800	-0.14510900
C	0.00001900	-1.40858200	1.20336700
H	-0.00001500	0.22984400	-2.92542600
H	-0.00002200	2.23111300	-1.90606400
H	-0.00003800	2.92542700	0.22984400
H	0.00002000	-1.90606400	-2.23111300
H	0.00003800	-2.92542700	-0.22984400
C	0.00000900	-0.14510900	1.84692700
H	-0.00001900	1.90606400	2.23111300
H	0.00001500	-0.22984400	2.92542600
H	0.00002200	-2.23111300	1.90606400
Ca	-2.09714500	-0.00001800	0.00000300
Ca	2.09714500	0.00001800	-0.00000300

State=1-A\MP2=-1662.5952478\S2=0.992005\S2-1=0.989023\S2A=0.005181

triplet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 3

C	-0.00001300	-1.69791800	0.74056500
C	-0.00004900	-0.67695100	1.72426700
C	-0.00006100	0.74056500	1.69791700
C	0.00003500	-1.72426900	-0.67695100
C	-0.00003500	1.72426900	0.67695100
C	0.00006000	-0.74056500	-1.69791700
C	0.00004900	0.67695100	-1.72426700
H	-0.00002500	-2.68956300	1.17308200
H	-0.00006400	-1.07231400	2.73130300
H	-0.00009500	1.17308100	2.68956300
H	0.00005200	-2.73130300	-1.07231400
H	0.00009400	-1.17308100	-2.68956300
C	0.00001300	1.69791800	-0.74056500
H	-0.00005200	2.73130300	1.07231500
H	0.00002500	2.68956400	-1.17308200
H	0.00006400	1.07231400	-2.73130200
Ca	2.09923600	0.00001000	0.00004400
Ca	-2.09923500	-0.00001000	-0.00004400

State=3-A\MP2=-1662.5940605\S2=2.000584\S2-1=2.000216\S2A=2.

5. The detailed Cartesian coordinates of $(DME)_3Ca\text{-}C_8H_8\text{-}Ca(DME)_3$ at PBEPBE/SVP level and PBEPBE/TZVPP//PBEPBE/SVP level

close-shell singlet $(DME)_3Ca\text{-}C_8H_8\text{-}Ca(DME)_3$

Charge = 0 Multiplicity = 1

C	-0.07454700	1.37441800	1.29669700
C	0.00093400	1.90146500	-0.02299200
C	0.07514600	1.34444200	-1.33022400
C	-0.09200100	0.06385500	1.85755000
C	0.09181900	0.02117100	-1.86070500
C	-0.09143100	-1.25841700	1.32535200
C	-0.00290000	-1.81906600	0.01958800
H	-0.12094600	2.16675500	2.07263300
H	0.00072300	3.01208800	-0.03560100
H	0.12058200	2.11867500	-2.12424200
H	-0.11696300	0.07952900	2.96801900
H	-0.13355900	-2.03637400	2.11751200
C	0.08882700	-1.28854900	-1.29863400
H	0.11606600	0.01146700	-2.97130000
H	0.13033900	-2.08418500	-2.07307100
H	-0.00497400	-2.92931000	0.03225000
O	-3.21496200	-1.66394300	-1.35509400
O	-3.70678200	-0.45057600	1.50897400
C	-3.53809600	-0.81054900	2.88134100
H	-2.45216200	-0.81212400	3.09466300
H	-4.04469700	-0.07057200	3.54277200
H	-3.95607200	-1.82547000	3.07254200
C	-5.07611300	-0.41459200	1.11179700
H	-5.64391000	0.32192500	1.72625700
H	-5.10753700	-0.10804600	0.04708100
H	-5.54416800	-1.42028200	1.22072700
C	-3.59063100	2.91078700	0.65886300
H	-4.59997100	3.36471800	0.52646100
H	-3.58251800	2.29070700	1.57846800
H	-2.82940800	3.71678500	0.75904300
C	-3.30002100	2.74236000	-1.69358900
H	-3.07484600	1.99874200	-2.48828200
H	-4.30607400	3.18493200	-1.87886100
H	-2.52397400	3.54160500	-1.71709500
C	-3.26923000	-2.99097900	-0.83431600
H	-3.12102800	-2.93028300	0.26350200
H	-4.26080500	-3.45180600	-1.04881400
H	-2.46345300	-3.62182800	-1.27275300
C	-3.43732800	-1.61706600	-2.76390800
H	-4.44037900	-2.03760300	-3.01120000
H	-3.39917600	-0.55099300	-3.07435300
H	-2.64627900	-2.18032800	-3.31043100
Ca	-1.96363600	0.04072700	-0.13155500
O	-3.28372100	2.05586800	-0.44182000
O	3.21637500	-1.65730100	1.35885000

O	3.71087800	-0.44372600	-1.50714600
C	3.54584600	-0.81988900	-2.87569900
H	2.46073300	-0.81684900	-3.09352600
H	4.06033000	-0.09159600	-3.54387500
H	3.95763500	-1.83997000	-3.05243700
C	5.07890900	-0.40866000	-1.10502700
H	5.65200100	0.31713300	-1.72725400
H	5.10752800	-0.08786400	-0.04449500
H	5.54303600	-1.41769000	-1.19867500
C	3.58235700	2.90908600	-0.66501200
H	4.58830500	3.37013800	-0.53139500
H	3.58176300	2.28374600	-1.58102000
H	2.81670500	3.70994900	-0.77259000
C	3.28645100	2.75158000	1.68732900
H	3.05985700	2.01186700	2.48517500
H	4.29068900	3.19777300	1.87389100
H	2.50856300	3.54919700	1.70382100
C	3.27116000	-2.98718900	0.84541200
H	3.11061000	-2.93388500	-0.25112900
H	4.26712800	-3.44229600	1.05168200
H	2.47291600	-3.61876900	1.29644200
C	3.45529100	-1.60055700	2.76461100
H	4.46658700	-2.00712600	3.00162800
H	3.40697400	-0.53356300	3.07035900
H	2.67806900	-2.17102800	3.32328500
Ca	1.96174500	0.03727600	0.12952100
O	3.27657600	2.05844600	0.43926900

PBEPBE/SVP State=1-A\HF=-2591.9731521
PBEPBE/TZVPP//PBEPBE/SVP State=1-A\HF=-2593.5127124

open-shell singlet $(DME)_3Ca\text{-}C_8H_8\text{-}Ca(DME)_3$
Charge = 0 Multiplicity = 1

C	0.07505200	1.35980600	-1.31328800
C	0.00005600	1.90162600	0.00036900
C	-0.07492300	1.35915000	1.31375500
C	0.09133300	0.04288700	-1.85933000
C	-0.09118500	0.04195500	1.85913500
C	0.08966300	-1.27333300	-1.31250800
C	0.00009100	-1.81922500	-0.00056400
H	0.12102000	2.14334700	-2.09811600
H	-0.00009400	3.01231300	0.00064700
H	-0.12105400	2.14230300	2.09896300
H	0.11535800	0.04613700	-2.96995700
H	0.13078100	-2.05993400	-2.09612400
C	-0.08951000	-1.27399100	1.31166000
H	-0.11524700	0.04465700	2.96976600
H	-0.13073100	-2.06097800	2.09488700
H	0.00002600	-2.92953900	-0.00084500

O	3.21644000	-1.66440900	1.34864900
O	3.70954100	-0.44251700	-1.50959000
C	3.54298700	-0.80790700	-2.88087500
H	2.45739600	-0.80839300	-3.09621500
H	4.05230500	-0.07157100	-3.54421300
H	3.95939700	-1.82442200	-3.06702300
C	5.07824800	-0.40629800	-1.11003300
H	5.64788800	0.32657700	-1.72711900
H	5.10798800	-0.09453300	-0.04682100
H	5.54535500	-1.41302200	-1.21324300
C	3.58742900	2.91191500	-0.64754900
H	4.59554200	3.36792800	-0.51284200
H	3.58274600	2.29211700	-1.56737200
H	2.82486100	3.71646700	-0.74927100
C	3.29158900	2.74220700	1.70408400
H	3.06212200	1.99882900	2.49768900
H	4.29733200	3.18380300	1.89345700
H	2.51639100	3.54234600	1.72458200
C	3.27138500	-2.99094600	0.82678300
H	3.11583400	-2.93031800	-0.27003600
H	4.26571400	-3.44898000	1.03458400
H	2.47027600	-3.62435700	1.27010000
C	3.44575000	-1.61797800	2.75637000
H	4.45252300	-2.03288900	2.99805000
H	3.40268000	-0.55260900	3.06851500
H	2.66079800	-2.18661000	3.30609200
Ca	1.96259000	0.03978700	0.12876900
O	3.27969100	2.05605600	0.45217000
O	-3.21615300	-1.66469200	-1.34839200
O	-3.70939500	-0.44206100	1.50963700
C	-3.54286000	-0.80783600	2.88082900
H	-2.45728900	-0.80801300	3.09627400
H	-4.05251200	-0.07188800	3.54433800
H	-3.95892900	-1.82455900	3.06660300
C	-5.07808700	-0.40614900	1.10998500
H	-5.64795600	0.32650200	1.72712700
H	-5.10783400	-0.09425900	0.04680900
H	-5.54494400	-1.41300600	1.21303500
C	-3.58798700	2.91190600	0.64747100
H	-4.59632100	3.36736800	0.51252600
H	-3.58312000	2.29224200	1.56738000
H	-2.82586500	3.71688200	0.74919000
C	-3.29147400	2.74204900	-1.70406600
H	-3.06138800	1.99870100	-2.49752200
H	-4.29739100	3.18309700	-1.89380500
H	-2.51668000	3.54258600	-1.72442200
C	-3.27140900	-2.99115400	-0.82640500
H	-3.11480600	-2.93058300	0.27026900
H	-4.26618800	-3.44864100	-1.03328200

H	-2.47106200	-3.62504400	-1.27042100
C	-3.44653000	-1.61820800	-2.75593200
H	-4.45399400	-2.03195100	-2.99676200
H	-3.40239700	-0.55294600	-3.06829100
H	-2.66268400	-2.18787000	-3.30616700
Ca	-1.96247900	0.03983200	-0.12895500
O	-3.27959600	2.05605900	-0.45205700

PBEPBE/SVP State=1-A\HF=-2591.9731594\S2=0.\S2-1=0.\S2A=0.
PBEPBE/TZVPP//PBEPBE/SVP State=1-A\HF=-2593.512712\S2=0.\S2-1=0.\S2A=0.

triplet $(DME)_3Ca\text{-}C_8H_8\text{-}Ca(DME)_3$
Charge = 0 Multiplicity = 3

C	-0.21044100	1.43465600	1.29895000
C	-0.00062800	1.97633800	0.00045300
C	0.20958200	1.43530500	-1.29825300
C	-0.31700000	0.11955800	1.83630000
C	0.31702400	0.12042200	-1.83604600
C	-0.24799600	-1.19395300	1.29222000
C	0.00005800	-1.73569800	-0.00026100
H	-0.30497500	2.21398500	2.07316500
H	-0.00075600	3.07960100	0.00069300
H	0.30411400	2.21497500	-2.07212300
H	-0.45833500	0.12179500	2.93048000
H	-0.36529200	-1.97763200	2.06110200
C	0.24813600	-1.19335300	-1.29250700
H	0.45897800	0.12312000	-2.93014400
H	0.36584600	-1.97666300	-2.06169400
H	0.00018200	-2.83889000	-0.00052100
O	-3.01405900	-1.94171300	-1.44169400
O	-3.85675100	-0.47845700	1.11932700
C	-3.78516500	-0.90331000	2.47362100
H	-2.71493400	-0.93177000	2.75159700
H	-4.32515300	-0.19395800	3.14296900
H	-4.23102400	-1.91752300	2.59800900
C	-5.19294000	-0.39163500	0.63090000
H	-5.78331500	0.34386800	1.22529500
H	-5.14111800	-0.05197300	-0.42611900
H	-5.69411900	-1.38659700	0.67486500
C	-3.42209000	2.86048500	1.19529600
H	-4.45933800	3.24174800	1.34117900
H	-3.20111100	2.08861400	1.95767700
H	-2.70721100	3.70500600	1.32199200
C	-3.54381000	3.16495200	-1.15390400
H	-3.44941400	2.58038600	-2.09569900
H	-4.57716000	3.57692900	-1.07183100

H	-2.80664500	4.00160800	-1.15098900
C	-3.09917800	-3.17828200	-0.75009500
H	-2.94996900	-2.97282600	0.32786600
H	-4.09814400	-3.64875000	-0.90465800
H	-2.31144500	-3.88699000	-1.09339000
C	-3.16665500	-2.08329000	-2.85330600
H	-4.15321800	-2.54433200	-3.09453900
H	-3.12191700	-1.05712300	-3.28111900
H	-2.34695400	-2.70895300	-3.27819900
Ca	-2.06000600	0.14304900	-0.49060900
O	-3.28454100	2.25726400	-0.08346100
O	3.01573100	-1.94012600	1.44189100
O	3.85677000	-0.47822800	-1.11934100
C	3.78659400	-0.90245600	-2.47388400
H	2.71666100	-0.93053200	-2.75309600
H	4.32753900	-0.19297300	-3.14231700
H	4.23225800	-1.91677000	-2.59822600
C	5.19244600	-0.39094400	-0.62961000
H	5.78280400	0.34566500	-1.22265300
H	5.13941900	-0.05246400	0.42772700
H	5.69440000	-1.38549400	-0.67420100
C	3.42188200	2.86063300	-1.19518700
H	4.45936100	3.24146900	-1.34051600
H	3.20079700	2.08925600	-1.95805000
H	2.70743800	3.70555500	-1.32168100
C	3.54332500	3.16393900	1.15411200
H	3.44827800	2.57912500	2.09568900
H	4.57699900	3.57516700	1.07239000
H	2.80674600	4.00111900	1.15136700
C	3.10053400	-3.17728600	0.75127000
H	2.95207600	-2.97253600	-0.32694400
H	4.09915400	-3.64818500	0.90673000
H	2.31220300	-3.88527700	1.09467200
C	3.16805900	-2.08070400	2.85363100
H	4.15481900	-2.54107800	3.09538300
H	3.12263100	-1.05432300	3.28086200
H	2.34859300	-2.70654000	3.27873800
Ca	2.05869700	0.14266200	0.48892700
O	3.28360100	2.25684500	0.08324200

PBEPBE/SVP State=3-A\HF=-2591.9678205\S2=2.00055\S2-1=0.\S2A=2.
PBEPBE/TZVPP//PBEPBE/SVP State=3-A\HF=-2593.5138758\S2=2.000638\S2-1=0.\S2A=2.

6. The detailed Cartesian coordinates of Ca-C_8H_8-Ca obtained at PBEPBE/SVP

close-shell singlet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 1

C	0.00002000	-1.72668200	-0.72123500
C	0.00005200	-0.71100500	-1.73088500
C	0.00007000	0.72123500	-1.72668000
C	-0.00003800	-1.73088700	0.71100500
C	0.00003900	1.73088700	-0.71100500
C	-0.00006900	-0.72123500	1.72668100
C	-0.00005100	0.71100500	1.73088500
H	0.00003700	-2.74260900	-1.14537300
H	0.00006100	-1.12908000	-2.74932700
H	0.00010600	1.14537300	-2.74260800
H	-0.00005500	-2.74932900	1.12908200
H	-0.00010500	-1.14537200	2.74260800
C	-0.00001900	1.72668200	0.72123500
H	0.00005500	2.74932900	-1.12908100
H	-0.00003500	2.74260900	1.14537400
H	-0.00006000	1.12908000	2.74932800
Ca	-2.17277700	0.00000900	-0.00004800
Ca	2.17277500	-0.00000900	0.00004700

State=1-A\HF=-1663.5275859

open-shell singlet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 1

C	-0.00002000	1.68913100	-0.80526200
C	-0.00005200	0.62503900	-1.76375100
C	-0.00007000	-0.80526200	-1.68912900
C	0.00003700	1.76375300	0.62503900
C	-0.00003900	-1.76375300	-0.62503800
C	0.00006900	0.80526200	1.68913000
C	0.00005100	-0.62503900	1.76375100
H	-0.00003800	2.68297400	-1.27884000
H	-0.00006100	0.99253200	-2.80151800
H	-0.00010600	-1.27884000	-2.68297300
H	0.00005400	2.80152000	0.99253400
H	0.00010500	1.27883900	2.68297400
C	0.00001900	-1.68913100	0.80526300
H	-0.00005500	-2.80152000	-0.99253300
H	0.00003500	-2.68297400	1.27884100
H	0.00006000	-0.99253200	2.80151900
Ca	2.17277700	-0.00001100	-0.00004700
Ca	-2.17277500	0.00001100	0.00004700

State=1-A\HF=-1663.5336513\S2=0.770733\S2-1=0.\S2A=0.000827

triplet Ca-C_8H_8-Ca

Charge = 0 Multiplicity = 3

C	-0.00002600	-0.86421500	1.65759200
C	-0.00040700	-1.78335500	0.56114200
C	-0.00031800	-1.65765600	-0.86418200
C	0.00020000	0.56116600	1.78325700
C	-0.00020000	-0.56116600	-1.78325700
C	0.00031800	1.65765600	0.86418200
C	0.00040700	1.78335500	-0.56114200
H	-0.00002000	-1.37305700	2.63400900
H	-0.00036700	-2.83358200	0.89169500
H	-0.00092100	-2.63410800	-1.37291600
H	-0.00015600	0.89184500	2.83343800
H	0.00092000	2.63410700	1.37291600
C	0.00002600	0.86421500	-1.65759200
H	0.00015600	-0.89184500	-2.83343800
H	0.00002000	1.37305700	-2.63400900
H	0.00036700	2.83358200	-0.89169500
Ca	-2.18519600	0.00026700	0.00006000
Ca	2.18519600	-0.00026700	-0.00006000

State=3-A\HF=-1663.5296884\S2=2.0002\S2-1=0.\S2A=2.