Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Characterizing a Nonclassical Carbene with Coupled Cluster Methods: Cyclobutylidene

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1 Data for Stationary Points

1.1 Cyclobutylidene ($\tilde{X}\ ^1A'$)

Software:	CFour 2.0beta
Theory:	CCSD(T)/ANO1
Reference:	RHF
CC Convergence:	10^{-10}
SCF Convergence:	10^{-10}
Charge:	0
Multiplicity:	1
Frozen Core:	ON
Geometry Convergence:	10^{-5} H/bohr
Total Energy (Hartree):	-155.594702317326

Equilibrium Geometry (Angstrom):

C	-0.8529669907	-0.3914546894	-0.0000000000
C	0.9205660398	-0.2226172167	-0.0000000000
C	-0.1427918976	0.2464763319	1.1117865036
C	-0.1427918976	0.2464763319	-1.1117865036
H	1.2572111956	-1.2489650900	-0.0000000000
H	1.7317189418	0.4961681670	0.0000000000
H	-0.1714568312	-0.2359267495	2.0834656680
H	-0.0252546932	1.3333982041	1.1645348759
H	-0.1714568312	-0.2359267495	-2.0834656680
H	-0.0252546932	1.3333982041	-1.1645348759

1.2 Cyclobutylidene ($\tilde{a}\ ^3A_1$)

Software:	CFour 2.0beta
Theory:	CCSD(T)/ANO1
Reference:	UHF
CC Convergence:	10^{-10}
SCF Convergence:	10^{-10}
Charge:	0
Multiplicity:	3
Frozen Core:	ON
Geometry Convergence:	10^{-5} H/bohr
Total Energy (Hartree):	-155.580921846141

Equilibrium Geometry (Angstrom):

C	-0.0000000000	0.0000000000	1.0730525334
C	-0.0000000000	-1.1361013673	0.0843474297
C	-0.0000000000	0.0000000000	-0.9977066363
C	0.0000000000	1.1361013673	0.0843474297
H	0.8884932100	-1.7727242571	0.0838334081
H	-0.8884932100	-1.7727242571	0.0838334081
H	-0.8932946627	0.0000000000	-1.6205425325
H	0.8932946627	0.0000000000	-1.6205425325
H	0.8884932100	1.7727242571	0.0838334081
H	-0.8884932100	1.7727242571	0.0838334081

1.3 TS1

Software:	CFour 2.0beta
Theory:	CCSD(T)/ANO1
Reference:	RHF
CC Convergence:	10^{-8}
SCF Convergence:	10^{-9}
Charge:	0
Multiplicity:	1
Frozen Core:	ON
Geometry Convergence:	10^{-7} H/bohr
Total Energy (Hartree):	-155.580762660452

Equilibrium Geometry (Angstrom):

C	-0.2056483280	-0.4775275650	-0.5747638262
C	0.4311375166	0.9126016947	-0.0377887167
C	1.0245921267	-0.4886532044	0.2326110836
C	-1.2833843711	-0.0855739303	0.2028305544
H	0.7674596626	1.5843909897	-0.8174867039
H	0.1697674117	1.4062287154	0.9003997881
H	1.9452584879	-0.7192786033	-0.2918525031
H	1.0327126638	-0.7393999226	1.2977901634
H	-2.1163562830	0.4440842719	-0.2529756868
H	-1.4023081100	-0.3191544613	1.2729541394

1.4 TS2

Software:	CFour 2.0beta
Theory:	CCSD(T)/ANO1
Reference:	RHF
CC Convergence:	10^{-8}
SCF Convergence:	10^{-9}
Charge:	0
Multiplicity:	1
Frozen Core:	ON
Geometry Convergence:	10^{-7} H/bohr
Total Energy (Hartree):	-155.577163197415

Equilibrium Geometry (Angstrom):

C	-0.9325570005	0.6771482995	0.0627240778
C	0.8284503304	-0.6955444481	0.0037014520
C	0.6178603072	0.8518225020	-0.0176156015
C	-0.6866393210	-0.7362102803	0.0221073956
H	1.2866497070	-1.0908740537	0.9121658960
H	1.3215154179	-1.1403833638	-0.8617302559
H	0.9758962679	1.3627278214	0.8779835699
H	0.9920774921	1.3850949478	-0.8921389767
H	-1.3921666238	-1.5624166028	0.1029618480
H	-1.1254520456	-0.1116838638	-0.9836425497

1.5 TS3

Software:	CFour 2.0beta
Theory:	CCSD(T)/ANO1
Reference:	RHF
CC Convergence:	10^{-8}
SCF Convergence:	10^{-9}
Charge:	0
Multiplicity:	1
Frozen Core:	ON
Geometry Convergence:	10^{-7} H/bohr
Total Energy (Hartree):	-155.572068566165

Equilibrium Geometry (Angstrom):

C	0.0000000053	-0.8749905381	-0.4429932408
C	-0.0000000000	0.8455742839	-0.2356454283
C	1.0852909586	-0.0665851561	0.3071999292
C	-1.0852909586	-0.0665851614	0.3071999239
H	-0.0000000000	0.3902466253	-1.3355085154
H	-0.0000000265	1.9122449662	-0.4317329363
H	2.0804518607	-0.0332694848	-0.1241818662
H	1.0629339448	-0.1500310636	1.3902428899
H	-2.0804518607	-0.0332695006	-0.1241818662
H	-1.0629339395	-0.1500310689	1.3902428846

1.6 P1 (Methylenecyclopropane)

Software:	CFour 2.0beta
Theory:	CCSD(T)/ANO1
Reference:	RHF
CC Convergence:	10^{-10}
SCF Convergence:	10^{-10}
Charge:	0
Multiplicity:	1
Frozen Core:	ON
Geometry Convergence:	10^{-5} H/bohr
Total Energy (Hartree):	-155.681445080385

Equilibrium Geometry (Angstrom):

C	-0.3063757409	-0.0000054558	0.0000000000
C	0.9440360668	-0.7722118913	0.0000000000
C	0.9440260601	0.7722171725	0.0000000000
C	-1.6320236097	-0.0000014182	-0.0000000000
H	1.2453372519	-1.2692974029	-0.9142429009
H	1.2453372519	-1.2692974029	0.9142429009
H	1.2453208104	1.2693065894	0.9142429009
H	1.2453208104	1.2693065894	-0.9142429009
H	-2.1909825573	-0.9282368609	-0.0000000000
H	-2.1909769004	0.9282374324	0.0000000000

1.7 P2 (Cyclobutene)

Software:	CFour 2.0beta
Theory:	CCSD(T)/ANO1
Reference:	RHF
CC Convergence:	10^{-10}
SCF Convergence:	10^{-10}
Charge:	0
Multiplicity:	1
Frozen Core:	ON
Geometry Convergence:	10^{-5} H/bohr
Total Energy (Hartree):	-155.694585914811

Equilibrium Geometry (Angstrom):

C	-0.6729464575	0.0000000000	-0.7904844399
C	-0.7855006750	0.0000000000	0.7267886286
C	0.7855006750	0.0000000000	0.7267886286
C	0.6729464575	0.0000000000	-0.7904844399
H	-1.2405906219	-0.8894931486	1.1671770314
H	-1.2405906219	0.8894931486	1.1671770314
H	1.2405906219	0.8894931486	1.1671770314
H	1.2405906219	-0.8894931486	1.1671770314
H	-1.4180911760	-0.0000000000	-1.5759389548
H	1.4180911760	0.0000000000	-1.5759389548

1.8 P3 (Bicylco[1.1.0]butane)

Software:	CFour 2.0beta
Theory:	CCSD(T)/ANO1
Reference:	RHF
CC Convergence:	10^{-10}
SCF Convergence:	10^{-10}
Charge:	0
Multiplicity:	1
Frozen Core:	ON
Geometry Convergence:	10^{-5} H/bohr
Total Energy (Hartree):	-155.669459413780

Equilibrium Geometry (Angstrom):

C	-0.0000000635	0.7486501949	-0.3186296709
C	-0.0000000053	-0.7486354679	-0.3186473666
C	1.1341167727	-0.0000058474	0.3163502240
C	-1.1341172596	-0.0000059427	0.3163494885
H	0.0000041752	1.4197537239	-1.1593028316
H	0.0000042916	-1.4197191263	-1.1593363867
H	2.0797287717	-0.0000099750	-0.2151439428
H	-2.0797289093	-0.0000101443	-0.2151453027
H	1.2187830370	-0.0000250883	1.4017153415
H	-1.2187847992	-0.0000243527	1.4017145054