Supplementary Materials

1.Cartesian coordinates of ground-state ethylene optimized at CCSD/aug-cc-pVDZ level

C	0.00000000	0.00000000	0.67443300
H	0.00000000	0.93325900	1.24746000
H	0.00000000	-0.93325900	1.24746000
C	0.00000000	0.00000000	-0.67443300
H	0.00000000	-0.93325900	-1.24746000
H	0.00000000	0.93325900	-1.24746000

(in Angstrom unit)

2.Optimized geometry of S1 state for ethylene calculated at CAM-B3LYP/aug-cc-pVTZ level

C	0.00000000	0.00000000	0.69139600
H	0.19349800	0.91771800	1.23734100
H	-0.19349800	-0.91771800	1.23734100
C	0.00000000	0.00000000	-0.69139600
H	0.19349800	-0.91771800	-1.23734100
H	-0.19349800	0.91771800	-1.23734100

3.Optimized geometry of S4 state for ethylene calculated at CAM-B3LYP/aug-cc-pVTZ level

C	0.00000000	0.00000000	0.69312800
H	0.19686800	0.90101100	1.26800600
H	-0.19686800	-0.90101100	1.26800600
C	0.00000000	0.00000000	-0.69312800
H	0.19686800	-0.90101100	-1.26800600
H	-0.19686800	0.90101100	-1.26800600

4.Optimized geometry of S5 state for ethylene calculated at CAM-B3LYP/aug-cc-pVTZ level

C	0.68495000	-0.00653200	0.00034100
H	1.16630800	1.00673800	-0.00069100

H	1.40702800	-0.81545000	-0.00124900
C	-0.68496600	0.00650600	0.00026800
H	-1.16636400	-1.00670800	-0.00059000
H	-1.40687900	0.81557200	-0.00112000

5.Optimized geometry of S6 state for ethylene calculated at CAM-B3LYP/aug-cc-pVTZ level

C	0.67788700	-0.00001700	-0.00001200
H	1.23568400	0.87378600	-0.32376700
H	1.23577500	-0.87366500	0.32383600
C	-0.67788600	0.00001700	-0.00001100
H	-1.23568700	-0.87378400	-0.32376900
H	-1.23577700	0.87366400	0.32383600

6.Optimized geometry of S7 state for ethylene calculated at CAM-B3LYP/aug-cc-pVTZ level

C	0.00000000	0.00000000	0.70287500
H	0.00000000	0.93056900	1.25052400
H	0.00000000	-0.93056900	1.25052400
C	0.00000000	0.00000000	-0.70287500
H	0.00000000	-0.93056900	-1.25052400
H	0.00000000	0.93056900	-1.25052400

7.Optimized geometry of S8 state for ethylene calculated at CAM-B3LYP/aug-cc-pVTZ level

C	0.00000000	0.00000000	0.69321000
H	0.17129900	0.93209200	1.22308100
H	-0.17129900	-0.93209200	1.22308100
C	0.00000000	0.00000000	-0.69321000
H	0.17129900	-0.93209200	-1.22308100
H	-0.17129900	0.93209200	-1.22308100

8.Optimized geometry of S9 state for ethylene calculated at CAM-B3LYP/aug-cc-pVTZ level

C	-0.00000900	-0.66316400	0.00000000

H	-0.92106700	-1.26088400	0.00000000
H	0.92116600	-1.26074000	0.00000000
C	-0.00000900	0.60007700	0.00000000
H	0.77876700	1.45007600	0.00000000
H	-0.77876300	1.45006800	0.00000000

9.Optimized geometry of S11 state for ethylene calculated at CAM-B3LYP/aug-cc-pVTZ level

C	0.00000000	0.00000000	0.69953100
H	0.07832000	0.96102300	1.22342500
H	-0.07832000	-0.96102300	1.22342500
C	0.00000000	0.00000000	-0.69953100
H	0.07832000	-0.96102300	-1.22342500
H	-0.07832000	0.96102300	-1.22342500

10.Optimized geometry of S14 state for ethylene calculated at CAM-B3LYP/aug-cc-pVTZ level

6	0.628659	0.015994	-0.000001
1	1.435012	0.762751	0.000004
1	1.098458	-1.051372	0.000007
6	-0.628659	-0.015994	-0.000002
1	-1.435012	-0.762751	0.000001
1	-1.098457	1.051372	0.000005

11.Optimized geometry of S15 state for ethylene calculated at CAM-B3LYP/aug-cc-pVTZ level

6	-0.000000	0.000000	0.629898
1	0.000000	0.847944	1.378707
1	-0.000000	-0.847944	1.378707
6	0.000000	0.000000	-0.629898
1	-0.000000	-0.847944	-1.378707
1	0.000000	0.847944	-1.378707

12.Optimized geometry of S16 state for ethylene calculated at CAM-B3LYP/aug-cc-pVTZ level

6	0.000000	0.692777	0.000000
1	0.155379	1.207108	0.938302
1	-0.155378	1.207115	-0.938305
6	0.000000	-0.692777	0.000000
1	0.155378	-1.207115	-0.938305
1	-0.155379	-1.207108	0.938302

13.IOp keywords to specify CAMh-B3LYP functional in gaussian program

cam-b3lyp iop(3/120=0310000000) iop(3/119=0310000000)

14.IOp keywords to specify ωhPBE0 functional in gaussian program

pbepbe IOp(3/76=1000010000,3/77=1000010000) IOp(3/107=0200000000,3/108=0200000000) IOp(3/119=0250000000,3/120=0250000000) IOp(3/130=02500,3/131=02500)

15.Vertical excitation energies calculated at EOM-CCSD/aug-cc-pVTZ level

No.	State	VEE	exp.
1	B3U	7.344	7.11
2	B1U	7.9129	7.63
3	B1G	8.0026	7.8
4	B2G	8.0515	8
5	B1G	8.4628	
6	AG	8.7909	8.29
7	AU	9.1951	
8	B3U	9.2119	8.62
9	B3G	9.7467	
10	B2G	9.8773	
11	B3U	10.088	
12	B1U	10.2932	9.33
13	B1G	10.2952	9.34
msa	0.472	rms	0.572

16. Vertical excitation energies calculated at M06-2X/aug-cc-pVTZ level

No.	State	VEE	exp.
1	B3U	6.8684	7.11
2	B1U	7.3787	7.63
3	B1G	7.3944	7.8
4	B2G	7.4833	8
5	B1G	7.8885	
6	AG	8.3476	8.29
7	AU	8.4976	
8	B3U	8.5882	8.62

9	B2G	9.0474	
10	B3G	9.1673	
11	B3U	9.5892	
12	B1U	9.6291	9.33
13	B2G	9.7074	
14	B1G	9.7432	9.34
msa	-0.086	rms	0.318

17. Vertical excitation energies calculated at ωB97X-D/aug-cc-pVTZ level

No	State	VEE	exp
1	B3U	6.9718	7.11
2	B1U	7.3983	7.63
3	B1G	7.5661	7.8
4	B2G	7.643	8
5	B1G	8.032	
6	AG	8.3828	8.29
7	AU	8.5932	
8	B3U	8.8397	8.62
9	B3G	9.2564	
10	B2G	9.4063	
11	B3U	9.6163	
12	B1G	9.6808	9.34
13	B2G	9.7016	
14	B1U	9.7404	9.33
msa	0.013	rms	0.273

18. Vertical excitation energies calculated at LC-ωHPBE/aug-cc-pVTZ level

No.	State	VEE	exp.
1	B3U	7.4978	7.11
2	B1U	7.513	7.63
3	B1G	8.0501	7.8
4	B1G	8.1567	
5	B2G	8.2613	8
6	AG	8.8952	8.29
7	AU	9.3096	
8	B3U	9.3767	8.62
9	B2G	9.3919	
10	B3G	9.7012	
11	B3U	10.1681	
12	B1U	10.2487	9.33
13	B1G	10.318	9.34
msa	0.505	rms	0.616

19. Vertical excitation energies calculated at ωhPBE0/aug-cc-pVTZ level

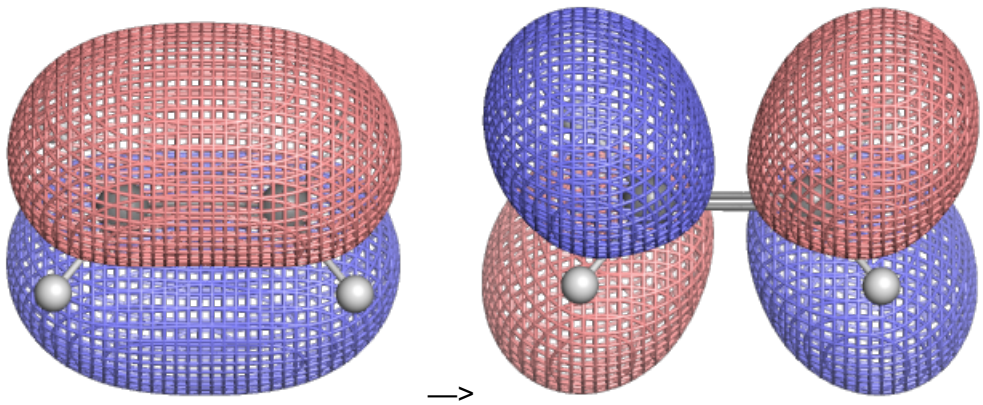
No.	State	VEE	exp.
1	B3U	6.8698	7.11

2	B1U	7.4075	7.63
3	B1G	7.4432	7.9
4	B2G	7.4704	8
5	B1G	7.9384	
6	AG	8.3635	8.29
7	AU	8.4512	
8	B3U	8.7121	8.62
9	B3G	9.0627	
10	B2G	9.382	
11	B3U	9.5049	
12	B2G	9.5365	
13	B1G	9.5785	9.34
14	B1U	9.6279	9.33
msa	-0.093	rms	0.307

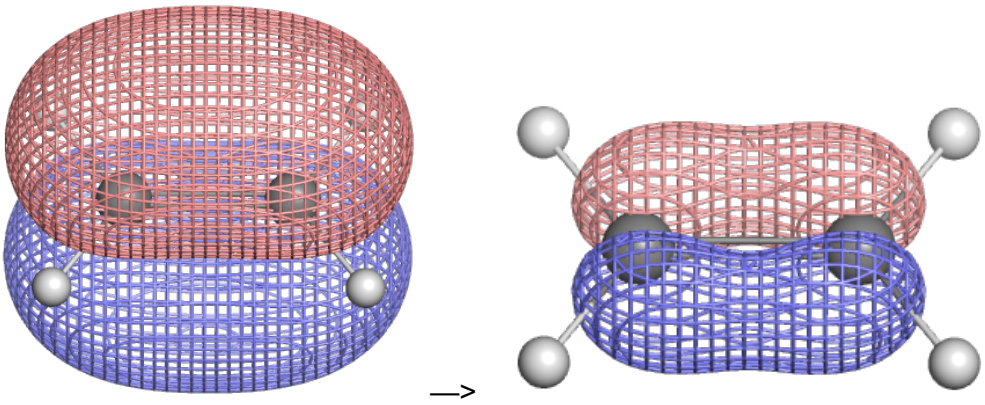
20. Vertical excitation energies calculated at CAMh-B3LYP/aug-cc-pVTZ level

No.	State	VEE	exp
1	B3U	6.7477	7.11
2	B1U	7.3132	7.63
3	B1G	7.3323	7.8
4	B2G	7.3623	8
5	B1G	7.98	
6	AG	8.2574	8.29
7	AU	8.3817	
8	B3U	8.5965	8.62
9	B3G	9.0576	
10	B2G	9.3707	
11	B3U	9.4144	
12	B2G	9.4767	
13	B1G	9.5016	9.34
14	B1U	9.5891	9.33
msa	-0.177	rms	0.345

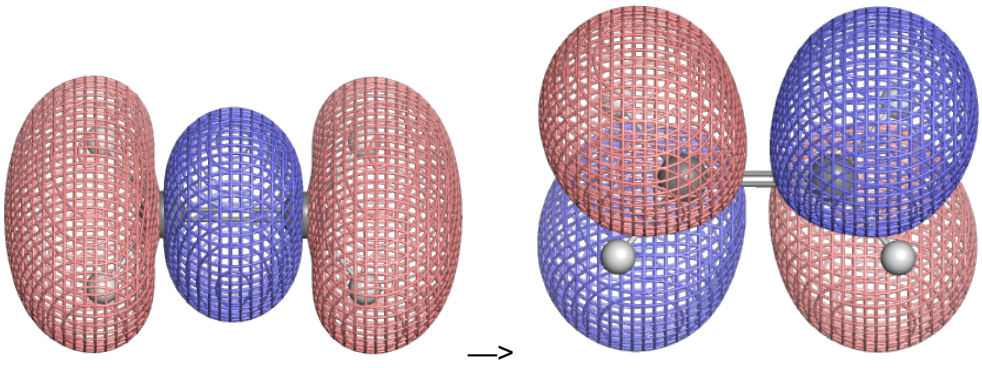
21. Natural transition orbitals digram for S2 state



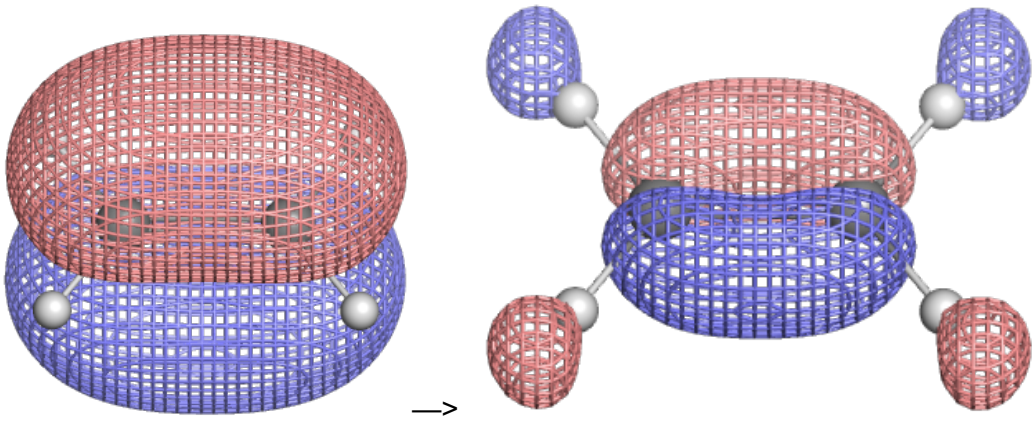
22. Natural transition orbitals diagram for S3 state



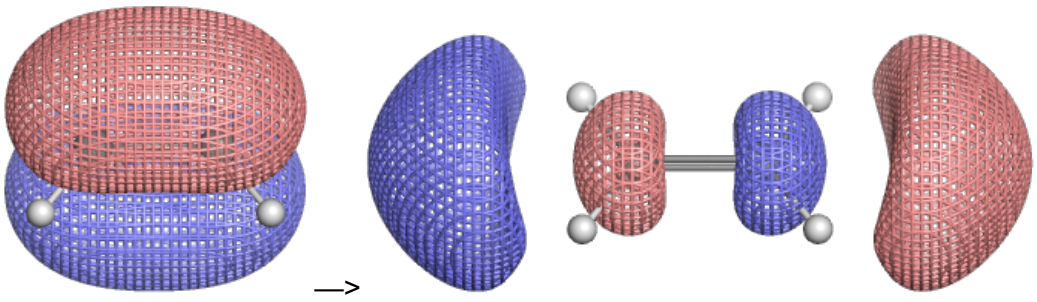
23. Natural transition orbitals diagram for S10 state



24.Natural transition orbitals diagram for S12 state

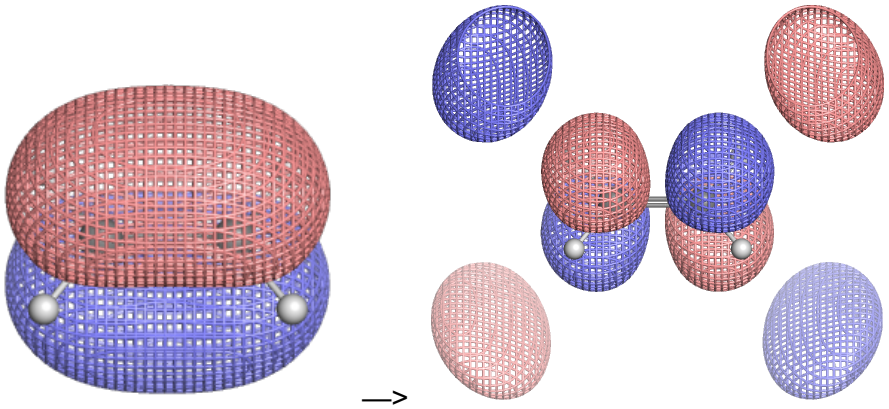


25. Natural transition orbitals diagram for S13 state



26. Natural transition orbitals diagram for S17 state

70%



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