Directing Power of Cyclobutenoid Annelations on the Double Bonds of Planar Cyclooctatetraenes

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(Supporting Information)

8 pages of optimized structural coordinate

Compound 5-exo

DZ(2d,p)	DZ(2df,pd)
-614.082761	-614.114296

C	0.781402	3.147435	-0.000450
C	-0.697545	1.716549	0.000170
C	-1.671164	0.800079	0.000120
C	0.800079	1.671164	-0.000160
C	-1.716558	-0.697541	-0.000190
C	-3.147435	0.781402	0.000260
C	1.716558	0.697541	-0.000150
C	-0.800079	-1.671164	-0.000180
C	-3.189007	-0.589462	-0.000340
H	-3.904300	1.555885	0.000900
C	1.671164	-0.800079	0.000210
C	3.189007	0.589462	-0.000350
C	0.697545	-1.716549	0.000170
C	-0.781402	-3.147435	-0.000220
H	-3.991432	-1.316645	-0.000970
C	3.147435	-0.781402	0.000420
H	3.991432	1.316645	-0.001260
C	0.589462	-3.189007	0.000190
H	3.904300	-1.555885	0.001320
C	-0.589462	3.189007	0.000500
H	1.555885	3.904300	-0.001550
H	-1.316645	3.991432	0.001600
H	-1.555885	-3.904300	-0.000670
H	1.316645	-3.991432	0.000650

Compound 6-exo

DZ(2d,p)	DZ(2df,pd)
-627.941548	-627.970577

H	-0.097353	3.990775	0.000000
N	0.468771	3.157452	0.000000
H	2.839075	3.412075	0.000000
C	1.376474	1.267460	0.000000
C	1.824825	0.000002	0.000000
C	0.000000	1.824816	0.000000
C	1.267451	-1.376461	0.000000
N	3.157453	-0.468791	0.000000
C	-1.267451	1.376461	0.000000
C	0.000000	-1.824818	0.000000
B	2.755578	-1.846884	0.000000
H	3.990788	0.097315	0.000000

C	-1.824824	-0.000003	0.000000
B	-2.755578	1.846883	0.000000
C	-1.376472	-1.267460	0.000000
N	-0.468773	-3.157452	0.000000
H	3.412038	-2.839102	0.000000
N	-3.157453	0.468790	0.000000
H	-3.412038	2.839101	0.000000
B	-1.846870	-2.755594	0.000000
H	0.097348	-3.990776	0.000000
H	-3.990787	-0.097317	0.000000
H	-2.839074	-3.412071	0.000000
B	1.846870	2.755599	0.000000

Compound 7-exo

DZ(2d,p)	DZ(2df,pd)
-979.323900	-979.367625

O	-1.613209	-4.051866	-0.000133
C	-1.551932	-2.857003	-0.000026
H	-3.573209	-1.861452	0.000254
C	-1.640877	-0.810979	0.000043
C	-0.526155	-1.769232	-0.000005
C	-1.769217	0.526153	-0.000029
C	0.810976	-1.640884	0.000045
C	-0.810976	1.640883	-0.000043
C	-2.856999	1.551932	-0.000016
C	1.769218	-0.526153	0.000036
N	1.848881	-2.564096	0.000056
C	0.526156	1.769232	0.000002
N	-1.848879	2.564097	-0.000022
O	-4.051863	1.613200	-0.000017
C	1.640877	0.810980	0.000023
C	2.856999	-1.551933	0.000006
H	1.861503	-3.573203	0.000081
C	1.551930	2.857003	0.000000
H	-1.861499	3.573204	0.000045
N	2.564101	1.848866	-0.000010
O	4.051863	-1.613201	-0.000043
O	1.613206	4.051867	0.000000
H	3.573208	1.861452	-0.000074
N	-2.564101	-1.848866	0.000121

Compound 8-exo (D4h)

DZ(2d,p)	DZ(2df,pd)
-747.012162	-747.057516

C	0.669067	1.725766	0.000000
C	-1.725766	0.669067	0.000000
C	-0.669067	-1.725766	0.000000
C	0.669067	-1.725766	0.000000
C	1.725766	0.669067	0.000000
C	-0.669067	1.725766	0.000000
C	-1.725766	-0.669067	0.000000
C	1.725766	-0.669067	0.000000
N	1.684527	2.699133	0.000000
N	-2.699133	1.684527	0.000000
N	-1.684527	-2.699133	0.000000
N	1.684527	-2.699133	0.000000
N	2.699133	1.684527	0.000000
N	-1.684527	2.699133	0.000000
N	-2.699133	-1.684527	0.000000
N	2.699133	-1.684527	0.000000
H	1.797045	3.691899	0.000000
H	-3.691899	1.797045	0.000000
H	-1.797045	-3.691899	0.000000
H	1.797045	-3.691899	0.000000
H	3.691899	1.797045	0.000000
H	-1.797045	3.691899	0.000000
H	-3.691899	-1.797045	0.000000
H	3.691899	-1.797045	0.000000

Compound 8-endo (D4h)

DZ(2d,p)	DZ(2df,pd)
-747.032461	-747.078503

C	0.694036	1.705077	0.000000
C	1.705077	-0.694036	0.000000
C	-0.694036	-1.705077	0.000000
C	-1.705077	-0.694036	0.000000
C	-0.694036	1.705077	0.000000
C	1.705077	0.694036	0.000000
C	0.694036	-1.705077	0.000000
C	-1.705077	0.694036	0.000000
N	0.699044	3.115627	0.000000
N	3.115627	-0.699044	0.000000
N	-0.699044	-3.115627	0.000000

N	-3.115627	-0.699044	0.000000
N	-0.699044	3.115627	0.000000
N	3.115627	0.699044	0.000000
N	0.699044	-3.115627	0.000000
N	-3.115627	0.699044	0.000000
H	1.324473	3.896282	0.000000
H	3.896282	-1.324473	0.000000
H	-1.324473	-3.896282	0.000000
H	-3.896282	-1.324473	0.000000
H	-1.324473	3.896282	0.000000
H	3.896282	1.324473	0.000000
H	1.324473	-3.896282	0.000000
H	-3.896282	1.324473	0.000000

Compound 8-I-exo (D4)

DZ(2d,p)	DZ(2df,pd)
-747.198779	-747.228494

C	-0.666904	1.706219	0.003729
C	1.706219	0.666904	0.003729
C	0.666904	-1.706219	0.003729
C	-0.666904	-1.706219	-0.003729
C	-1.706219	0.666904	-0.003729
C	0.666904	1.706219	-0.003729
C	1.706219	-0.666904	-0.003729
C	-1.706219	-0.666904	0.003729
N	-1.681892	2.728367	0.076572
N	2.728367	1.681892	0.076572
N	1.681892	-2.728367	0.076572
N	-1.681892	-2.728367	-0.076572
N	-2.728367	1.681892	-0.076572
N	1.681892	2.728367	-0.076572
N	2.728367	-1.681892	-0.076572
N	-2.728367	-1.681892	0.076572
H	-1.704813	3.313564	-0.759930
H	3.313564	1.704813	-0.759930
H	1.704813	-3.313564	-0.759930
H	-1.704813	-3.313564	0.759930
H	-3.313564	1.704813	0.759930
H	1.704813	3.313564	0.759930
H	3.313564	-1.704813	0.759930
H	-3.313564	-1.704813	-0.759930

Compound 8-I-endo (D4)

DZ(2d,p)	DZ(2df,pd)
-747.195647	-747.224178

C	-0.711013	-1.668935	0.103339
C	1.678844	-0.714569	-0.060271
C	0.711011	1.668907	0.103417
C	-0.709047	1.669742	-0.103297
C	-1.679689	-0.712605	0.060226
C	0.709049	-1.669772	-0.103379
C	1.679694	0.712563	0.060331
C	-1.678842	0.714538	-0.060294
N	-1.642949	-2.655073	0.588179
N	2.709963	-1.668013	-0.367481
N	1.643009	2.655300	0.587585
N	-1.639820	2.657061	-0.587912
N	-2.711951	-1.664860	0.367285
N	1.639831	-2.657038	-0.588096
N	2.711915	1.664741	0.367806
N	-2.709960	1.668016	-0.367404
H	-1.791688	-3.442532	-0.048042
H	3.174276	-1.501125	-1.263526
H	1.791986	3.442262	-0.049236
H	-1.787727	3.444528	0.048526
H	-3.176254	-1.497398	1.263232
H	1.787740	-3.444575	0.048254
H	3.175629	1.497461	1.264099
H	-3.174269	1.501234	-1.263471

Compound 9-exo

DZ(2d,p)	DZ(2df,pd)
-1211.023183	-1211.065662

C	2.817645	1.669178	0.000000
C	0.680488	1.697843	0.000000
C	-0.680488	1.697843	0.000000
C	1.697843	0.680488	0.000000
C	-1.697843	0.680488	0.000000
C	-1.669178	2.817645	0.000000
C	1.697843	-0.680488	0.000000
C	-1.697843	-0.680488	0.000000
C	-2.817645	1.669178	0.000000
O	-1.648028	4.003333	0.000000
C	0.680488	-1.697843	0.000000
C	2.817645	-1.669178	0.000000

C	-0.680488	-1.697843	0.000000
C	-2.817645	-1.669178	0.000000
O	-4.003333	1.648028	0.000000
C	1.669178	-2.817645	0.000000
O	4.003333	-1.648028	0.000000
C	-1.669178	-2.817645	0.000000
O	1.648028	-4.003333	0.000000
C	1.669178	2.817645	0.000000
O	4.003333	1.648028	0.000000
O	1.648028	4.003333	0.000000
O	-4.003333	-1.648028	0.000000
O	-1.648028	-4.003333	0.000000

Compound 9-endo

DZ(2d,p)	DZ(2df,pd)
-1211.031083	-1211.072027

C	0.686328	1.705618	0.000000
C	1.705618	-0.686328	0.000000
C	-0.686328	-1.705618	0.000000
C	-1.705618	-0.686328	0.000000
C	-0.686328	1.705618	0.000000
C	1.705618	0.686328	0.000000
C	0.686328	-1.705618	0.000000
C	-1.705618	0.686328	0.000000
C	0.782976	3.228784	0.000000
C	3.228784	-0.782976	0.000000
C	-0.782976	-3.228784	0.000000
C	-3.228784	-0.782976	0.000000
C	-0.782976	3.228784	0.000000
C	3.228784	0.782976	0.000000
C	0.782976	-3.228784	0.000000
C	-3.228784	0.782976	0.000000
O	1.663012	4.028908	0.000000
O	4.028908	-1.663012	0.000000
O	-1.663012	-4.028908	0.000000
O	-4.028908	-1.663012	0.000000
O	-1.663012	4.028908	0.000000
O	4.028908	1.663012	0.000000
O	1.663012	-4.028908	0.000000
O	-4.028908	1.663012	0.000000

Compound 10-endo

DZ(2d,p)	DZ(2df,pd)
-508.007914	-508.023574

C	0.701097	1.744182	0.000000
C	1.744182	-0.701097	0.000000
C	-0.701097	-1.744182	0.000000
C	-1.744182	-0.701097	0.000000
C	-0.701097	1.744182	0.000000
C	1.744182	0.701097	0.000000
C	0.701097	-1.744182	0.000000
C	-1.744182	0.701097	0.000000
B	0.850762	3.303577	0.000000
B	3.303577	-0.850762	0.000000
B	-0.850762	-3.303577	0.000000
B	-3.303577	-0.850762	0.000000
B	-0.850762	3.303577	0.000000
B	3.303577	0.850762	0.000000
B	0.850762	-3.303577	0.000000
B	-3.303577	0.850762	0.000000
H	1.832170	3.981507	0.000000
H	3.981507	-1.832170	0.000000
H	-1.832170	-3.981507	0.000000
H	-3.981507	-1.832170	0.000000
H	-1.832170	3.981507	0.000000
H	3.981507	1.832170	0.000000
H	1.832170	-3.981507	0.000000
H	-3.981507	1.832170	0.000000