J. Mex. Chem. Soc. **2024**, *68*(1)
Special Issue

ISSN-e 2594-0317

The Contribution of Dispersion to the Intrinsic Energy Barriers of Neutral Model Diels-Alder Reactions

Hugo Alejandro Jiménez-Vázquez*, Luis Almazán, Adriana Benavides

Departamento de Química Orgánica. Escuela Nacional de Ciencias Biológicas. Instituto Politécnico Nacional. Prol. Carpio y Plan de Ayala. Col. Plutarco Elías Calles. Ciudad de México, CP 11350. México.

***Corresponding author:** Hugo A. Jiménez-Vázquez, email: hjimenezv@ipn.mx; Tel: +52(55)5729-6000×62562.

Received June 30th, 2022; Accepted November 15th, 2022.

DOI for the article: http://dx.doi.org/10.29356/jmcs.v68i1.1867

Supplementary Information

J. Mex. Chem. Soc. **2024**, *68*(1)
Special Issue

ISSN-e 2594-0317

IRC of the 1+2 cycloaddition
SCS-MP2/*aug*-cc-pVTZ electronic energies in a.u.

Point -15 Energy= -0.23404283385253E+03

C	1.316162	-0.418305	-0.731870
C	1.316161	-0.418310	0.731868
H	2.182698	0.026037	1.209283
H	2.182699	0.026051	-1.209278
C	0.321695	-0.865327	-1.516890
C	0.321705	-0.865340	1.516894
C	-1.465445	1.218691	-0.667932
C	-1.465451	1.218703	0.667930
H	-2.178484	0.633426	-1.233850
H	-2.178481	0.633425	1.233856
H	-0.764463	1.816689	-1.232601
H	-0.764460	1.816697	1.232603
H	-0.562942	-1.335487	-1.111049
H	-0.562982	-1.335457	1.111026
H	0.391202	-0.792664	-2.593948
H	0.391211	-0.792687	2.593954

Point -14 Energy= -0.23404189214695E+03

C	1.311067	-0.414195	-0.731338
C	1.311067	-0.414196	0.731338
H	2.176817	0.029719	1.210493
H	2.176816	0.029719	-1.210494
C	0.310077	-0.853076	-1.513164
C	0.310075	-0.853075	1.513163
C	-1.448538	1.202211	-0.668070
C	-1.448538	1.202211	0.668070
H	-2.161963	0.617602	-1.234054
H	-2.161965	0.617606	1.234053
H	-0.750453	1.803408	-1.232756
H	-0.750451	1.803407	1.232754
H	-0.572076	-1.325372	-1.104792
H	-0.572061	-1.325386	1.104797
H	0.373385	-0.775955	-2.590287
H	0.373384	-0.775955	2.590287

Point -13 Energy= -0.23404081730067E+03

C	1.306524	-0.410545	-0.730729
C	1.306524	-0.410546	0.730729
H	2.171179	0.033314	1.211833
H	2.171179	0.033315	-1.211833
C	0.298306	-0.840449	-1.508861
C	0.298305	-0.840449	1.508861
C	-1.431904	1.185707	-0.668247
C	-1.431904	1.185707	0.668248
H	-2.146222	0.602309	-1.234279
H	-2.146222	0.602310	1.234278
H	-0.736986	1.790393	-1.232921
H	-0.736986	1.790393	1.232922
H	-0.580657	-1.315785	-1.097803
H	-0.580653	-1.315790	1.097803
H	0.354587	-0.758110	-2.586049
H	0.354587	-0.758112	2.586049

Point -12 Energy= -0.23403959735420E+03

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C	0.286418	-0.827470	-1.504034
C	0.286417	-0.827469	1.504034
C	-1.415533	1.169198	-0.668481
C	-1.415532	1.169199	0.668481
H	-2.131274	0.587682	-1.234494
H	-2.131273	0.587683	1.234496
H	-0.724128	1.777728	-1.233091
H	-0.724126	1.777727	1.233090
H	-0.588750	-1.306988	-1.090194
H	-0.588750	-1.306983	1.090191
H	0.334976	-0.739216	-2.581112
H	0.334975	-0.739218	2.581111

Point -11 Energy= -0.234038221729 91E+03

C	1.298920	-0.404594	-0.729223
C	1.298920	-0.404595	0.729224
H	2.160472	0.040382	1.214654
H	2.160471	0.040384	-1.214654
C	0.274421	-0.814157	-1.498702
C	0.274421	-0.814156	1.498702
C	-1.399405	1.152690	-0.668780
C	-1.399404	1.152690	0.668780
H	-2.117200	0.573741	-1.234732
H	-2.117200	0.573742	1.234733

C	1.302489	-0.407349	-0.730029
C	1.302490	-0.407350	0.730030
H	2.165728	0.036865	1.213236
H	2.165726	0.036868	-1.213236

H	0.273501	-0.677831	-2.562965
H	0.273501	-0.677830	2.562965

Point -8 Energy= -0.234033099195 64E+03

C	1.290541	-0.398664	-0.725928
C	1.290541	-0.398664	0.725928
H	2.146044	0.049952	1.218345
H	2.146045	0.049952	-1.218345
C	0.237906	-0.772211	-1.480201
C	0.237905	-0.772211	1.480200
C	-1.352195	1.103046	-0.670368
C	-1.352195	1.103045	0.670368
H	-2.081008	0.537538	-1.235274
H	-2.081007	0.537537	1.235276
H	-0.681229	1.734098	-1.233997
H	-0.681230	1.734099	1.233995
H	-0.614601	-1.282406	-1.057957
H	-0.614601	-1.282406	1.057956
H	0.253094	-0.656809	-2.555786
H	0.253093	-0.656809	2.555786

Point -7 Energy= -0.234031066365 28E+03

C	1.288401	-0.397321	-0.724419
C	1.288402	-0.397321	0.724420
H	2.141971	0.052338	1.219232
H	-0.711976	1.765617	-1.233295
H	-0.711975	1.765618	1.233294
H	-0.596172	-1.299037	-1.082218
H	-0.596172	-1.299037	1.082216
H	0.314751	-0.719379	-2.575651
H	0.314750	-0.719380	2.575651

Point -10 Energy= -0.234036682221 79E+03

C	1.295768	-0.402252	-0.728291
C	1.295768	-0.402253	0.728291
H	2.155398	0.043801	1.216013
H	2.155397	0.043802	-1.216012
C	0.262342	-0.800505	-1.492933
C	0.262342	-0.800505	1.492933
C	-1.383497	1.136173	-0.669175
C	-1.383496	1.136173	0.669175
H	-2.104016	0.560640	-1.234937
H	-2.104017	0.560642	1.234938
H	-0.700685	1.754168	-1.233500
H	-0.700684	1.754167	1.233499
H	-0.603044	-1.292228	-1.074006
H	-0.603045	-1.292226	1.074005
H	0.294163	-0.698831	-2.569494
H	0.294162	-0.698831	2.569494

Point -9 Energy= -0.234034974297 56E+03

C	1.292986	-0.400292	-0.727203
C	1.292986	-0.400292	0.727204
H	2.150581	0.047045	1.217269
H	2.150580	0.047047	-1.217269
C	0.250166	-0.786531	-1.486737
C	0.250165	-0.786531	1.486737
C	-1.367772	1.119632	-0.669684
C	-1.367771	1.119632	0.669684
H	-2.091932	0.548475	-1.235158
H	-2.091931	0.548475	1.235158
H	-0.638360	1.746318	-1.234337
H	-0.638361	1.746318	1.234334
H	-0.625289	-1.280517	-1.058482
H	-0.625290	-1.280518	1.058482
H	0.196931	-0.598055	-2.533505
H	0.196931	-0.598056	2.533506

Point -4 Energy= -0.234024352476 35E+03

C	1.283917	-0.394345	-0.717920
C	1.283917	-0.394345	0.717921
H	2.133597	0.054199	1.220205
H	2.133596	0.054199	-1.220206
C	0.187289	-0.711887	-1.451528
C	0.187289	-0.711887	1.451528
C	-1.290776	1.035985	-0.676413
C	-1.290777	1.035985	0.676413
H	-2.054267	0.511472	-1.234661
H	-2.054268	0.511473	1.234661
H	-0.660914	1.711991	-1.234926
H	-0.660914	1.711991	1.234926
H	-0.626782	-1.284806	-1.034206
H	-0.609116	-1.286540	1.065888

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H	2.141972	0.052338	-1.219231
C	0.225510	-0.757574	-1.473310
C	0.225510	-0.757574	1.473310
C	-1.336731	1.086399	-0.671260
C	-1.336731	1.086399	0.671260
H	-2.071530	0.527914	-1.235405
H	-2.071530	0.527915	1.235405
H	-0.673382	1.725879	-1.234313
H	-0.673380	1.725878	1.234313
H	-0.619087	-1.279682	-1.050634
H	-0.619087	-1.279684	1.050632
H	0.233278	-0.636135	-2.548549
H	0.233277	-0.636136	2.548548

Point -6 Energy= -0.23402889783898E+03

C	1.286573	-0.396198	-0.722620
C	1.286573	-0.396198	0.722620
H	2.138381	0.054003	1.219826
H	2.138380	0.054004	-1.219826
C	0.212983	-0.742594	-1.466209
C	0.212983	-0.742594	1.466209
C	-1.321346	1.069663	-0.672494
C	-1.321346	1.069664	0.672494
H	-2.063670	0.520176	-1.235312
H	-2.063669	0.520177	1.235312
H	-0.667278	1.719274	-1.234557
H	-0.667278	1.719274	1.234557
H	-0.622886	-1.279165	-1.043964
H	-0.622886	-1.279163	1.043963
H	0.214442	-0.616445	-2.540738
H	0.214441	-0.616446	2.540737

Point -5 Energy= -0.23402663574304E+03

C	1.285061	-0.395236	-0.720468
C	1.285061	-0.395237	0.720468
H	2.135608	0.054702	1.220193
H	2.135608	0.054702	-1.220193
C	0.200234	-0.727365	-1.458867
C	0.200234	-0.727365	1.458867
C	-1.306017	1.052845	-0.674150
C	1.283032	-0.391431	-0.707639
C	1.283032	-0.391431	0.707639
H	2.133386	0.045713	1.219301
H	2.133386	0.045713	-1.219301
C	0.146594	-0.665461	-1.430392
C	0.146594	-0.665460	1.430392
C	-1.246100	0.985854	-0.688281
C	-1.246100	0.985854	0.688281
H	-2.054606	0.515212	-1.232059
H	-2.054606	0.515213	1.232059
H	-0.664837	1.714578	-1.234200
H	-0.664837	1.714577	1.234200
H	-0.624787	-1.306268	-1.029524
H	-0.624787	-1.306268	1.029524
H	0.146529	-0.548670	-2.507493
H	-0.626781	-1.284804	1.034205
H	0.180924	-0.581690	-2.525689
H	0.180924	-0.581691	2.525690

Point -3 Energy= -0.23402216971029E+03

C	1.283254	-0.393436	-0.714873
C	1.283254	-0.393436	0.714873
H	2.132854	0.052413	1.220013
H	2.132853	0.052413	-1.220013
C	0.173929	-0.696433	-1.444218
C	0.173929	-0.696433	1.444218
C	-1.275647	1.019149	-0.679522
C	-1.275647	1.019149	0.679522
H	-2.053142	0.510919	-1.233962
H	-2.053143	0.510920	1.233962
H	-0.660841	1.711716	-1.234874
H	-0.660841	1.711715	1.234875
H	-0.626412	-1.291103	-1.031366
H	-0.626412	-1.291103	1.031365
H	0.166928	-0.567162	-2.519319
H	0.166927	-0.567162	2.519319

Point -2 Energy= -0.23402027716083E+03

C	1.282842	-0.392309	-0.711464
C	1.282843	-0.392309	0.711464
H	2.133581	0.047646	1.219669
H	2.133580	0.047645	-1.219670
C	0.160591	-0.681018	-1.437188
C	0.160591	-0.681018	1.437188
C	-1.260672	1.002403	-0.683331
C	-1.260672	1.002403	0.683331
H	-2.054067	0.513639	-1.232657
H	-2.054067	0.513640	1.232657
H	-0.663403	1.713672	-1.234333
H	-0.663403	1.713671	1.234332
H	-0.624504	-1.301131	-1.030400
H	-0.624503	-1.301131	1.030400
H	0.153185	-0.554606	-2.512238
H	0.153185	-0.554606	2.512238

Point -1 Energy= -0.23401894972383E+03

H	-0.682540	1.729300	-1.229407
H	-0.682537	1.729298	1.229403
H	-0.608871	-1.345016	-1.038467
H	-0.608873	-1.345015	1.038469
H	0.117193	-0.519641	-2.492120
H	0.117199	-0.519638	2.492120

Point 3 Energy= -0.23402424664239E+03

C	1.286726	-0.386432	-0.692275
C	1.286725	-0.386432	0.692274
H	2.147189	0.011324	1.218771
H	2.147192	0.011319	-1.218768
C	0.090427	-0.608246	-1.406275
C	0.090427	-0.608246	1.406274
C	-1.191793	0.923606	-0.714089
C	-1.191793	0.923606	0.714088

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H	0.146529	-0.548670	2.507493

Point TS Energy= -0.23401848504841E+03

C	1.2837666158	-0.3906629717	-0.7038387812
C	1.2837666136	-0.3906629696	0.7038387864
H	2.1366468864	0.0376644370	1.2187604271
H	2.1366468903	0.0376644335	-1.2187604205
C	0.1331530926	-0.6515600888	-1.4241771125
C	0.1331530881	-0.6515600847	1.4241771147
C	-1.2330319680	0.9709278674	-0.6937464849
C	-1.2330319702	0.9709278694	0.6937464782
H	-2.0604662675	0.5238772692	-1.2294853246
H	-2.0604662714	0.5238772727	1.2294853165
H	-0.6715370313	1.7205886575	-1.2327401230
H	-0.6715370352	1.7205886610	1.2327401159
H	-0.6186436254	-1.3218371638	-1.0321094367
H	-0.6186436286	-1.3218371609	1.0321094386
H	0.1337221199	-0.5358227157	-2.5015321545
H	0.1337221119	-0.5358227086	2.5015321564

Point 1 Energy= -0.23401905235430E+03

C	1.284766	-0.389662	-0.699986
C	1.284766	-0.389662	0.699987
H	2.140955	0.027621	1.218423
H	2.140953	0.027624	-1.218423
C	0.119489	-0.637859	-1.418217
C	0.119488	-0.637859	1.418217
C	-1.220111	0.956070	-0.699884
C	-1.220111	0.956070	0.699884
H	-2.066972	0.533991	-1.226287
H	-2.066972	0.533991	1.226287
H	-0.679065	1.727054	-1.230728
H	-0.679064	1.727054	1.230728
H	-0.611240	-1.338192	-1.036112
H	-0.611240	-1.338192	1.036111
H	0.121344	-0.523324	-2.495816
H	0.121343	-0.523324	2.495816

Point 2 Energy= -0.234020924338 83E+03

C	1.285800	-0.388291	-0.695993
C	1.285799	-0.388291	0.695992
H	2.143061	0.021974	1.218517
H	2.143067	0.021966	-1.218516
C	0.104789	-0.622829	-1.412144
C	0.104789	-0.622830	1.412145
C	-1.205994	0.939813	-0.706913
C	-1.205994	0.939813	0.706913
H	-2.069205	0.538831	-1.224514
H	-2.069206	0.538836	1.224519
H	2.160818	-0.025253	-1.221571
C	0.046078	-0.564636	-1.389042
C	0.046078	-0.564636	1.389043
C	-1.149690	0.874900	-0.736849
C	-1.149690	0.874900	0.736849
H	-2.080072	0.570438	-1.208462
H	-2.080072	0.570439	1.208463
H	-2.072844	0.547336	-1.221096
H	-2.072843	0.547338	1.221098
H	-0.688955	1.733544	-1.226749
H	-0.688954	1.733547	1.226747
H	-0.602771	-1.357635	-1.042709
H	-0.602775	-1.357637	1.042720
H	0.107914	-0.511934	-2.486301
H	0.107920	-0.511931	2.486300

Point 4 Energy= -0.23402904397203E+03

C	1.287848	-0.384466	-0.688665
C	1.287847	-0.384466	0.688664
H	2.151742	0.000139	1.219389
H	2.151746	0.000138	-1.219394
C	0.075641	-0.593830	-1.400415
C	0.075641	-0.593830	1.400416
C	-1.177707	0.907433	-0.721645
C	-1.177707	0.907434	0.721645
H	-2.076231	0.555407	-1.217313
H	-2.076231	0.555408	1.217314
H	-0.694649	1.737094	-1.223658
H	-0.694649	1.737094	1.223656
H	-0.595424	-1.368336	-1.047776
H	-0.595423	-1.368337	1.047779
H	0.100074	-0.504154	-2.482319
H	0.100076	-0.504151	2.482321

Point 5 Energy= -0.23403523294784E+03

C	1.288914	-0.382394	-0.685357
C	1.288913	-0.382394	0.685356
H	2.156232	-0.012075	1.220266
H	2.156233	-0.012077	-1.220265
C	0.060873	-0.579270	-1.394769
C	0.060873	-0.579270	1.394769
C	-1.163691	0.891219	-0.729307
C	-1.163690	0.891220	0.729307
H	-2.078603	0.563318	-1.213013
H	-2.078602	0.563319	1.213013
H	-0.699915	1.739532	-1.220030
H	-0.699914	1.739535	1.220029
H	-0.588579	-1.378942	-1.052985
H	-0.588578	-1.378943	1.052990
H	0.092627	-0.496671	-2.476968
H	0.092629	-0.496667	2.476968

Point 6 Energy= -0.23404260906393E+03

C	1.289783	-0.380232	-0.682405
C	1.289783	-0.380232	0.682404
H	2.160814	-0.025252	1.221572
H	-0.561771	-1.403426	1.075366
H	0.063432	-0.461234	-2.456934
H	0.063433	-0.461232	2.456935

Point 10 Energy= -0.23407803607833E+03

C	1.289671	-0.370564	-0.674591
C	1.289671	-0.370564	0.674591
H	2.176095	-0.087715	1.230541

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H	-0.704200	1.740764	-1.216021
H	-0.704199	1.740764	1.216020
H	-0.581116	-1.387586	-1.058727
H	-0.581115	-1.387587	1.058730
H	0.085447	-0.488869	-2.472406
H	0.085448	-0.488867	2.472407

Point 7 Energy= -0.23405088617898E+03

C	1.290367	-0.377979	-0.679862
C	1.290366	-0.377979	0.679861
H	2.165176	-0.039404	1.223232
H	2.165178	-0.039405	-1.223230
C	0.031406	-0.549797	-1.383335
C	0.031406	-0.549797	1.383335
C	-1.135687	0.858436	-0.744135
C	-1.135687	0.858436	0.744134
H	-2.080193	0.576447	-1.203657
H	-2.080193	0.576449	1.203657
H	-0.707239	1.740398	-1.211640
H	-0.707238	1.740398	1.211640
H	-0.574151	-1.394875	-1.064366
H	-0.574151	-1.394875	1.064369
H	0.078302	-0.480553	-2.467320
H	0.078304	-0.480550	2.467320

Point 8 Energy= -0.23405975326803E+03

C	1.290576	-0.375628	-0.677732
C	1.290576	-0.375628	0.677732
H	2.169274	-0.054517	1.225297
H	2.169276	-0.054518	-1.225297
C	0.016904	-0.534782	-1.377564
C	0.016905	-0.534781	1.377565
C	-1.121659	0.841800	-0.751025
C	-1.121659	0.841801	0.751025
H	-2.078939	0.581019	-1.198776
H	-2.078939	0.581020	1.198777
H	-0.708744	1.738334	-1.207022
H	-0.708744	1.738334	1.207021
H	-0.567570	-1.400113	-1.069976
H	-0.567569	-1.400113	1.069977
H	0.071015	-0.471404	-2.462225
H	0.071017	-0.471402	2.462227

Point 9 Energy= -0.23406890296514E+03

C	1.290359	-0.373165	-0.675993
C	1.290359	-0.373165	0.675993
H	2.172941	-0.070598	1.227735
H	2.172942	-0.070600	-1.227736
C	0.002661	-0.519588	-1.371763
C	0.002661	-0.519588	1.371764
C	-1.107601	0.824994	-0.757432
C	-1.107601	0.824995	0.757432
H	-2.076200	0.583939	-1.193926
H	-2.076199	0.583941	1.193926
H	-0.708577	1.734501	-1.202226
H	-0.708576	1.734501	1.202225
H	-0.561771	-1.403426	-1.075365
H	2.176096	-0.087716	-1.230543
C	-0.011260	-0.504265	-1.365956
C	-0.011260	-0.504265	1.365957
C	-1.093510	0.808031	-0.763275
C	-1.093509	0.808032	0.763275
H	-2.072026	0.585122	-1.189203
H	-2.072025	0.585124	1.189203
H	-0.706685	1.728970	-1.197292
H	-0.706684	1.728970	1.197291
H	-0.556846	-1.404745	-1.080544
H	-0.556846	-1.404745	1.080545
H	0.055454	-0.449883	-2.451526
H	0.055455	-0.449881	2.451526

Point 11 Energy= -0.23408685302390E+03

C	1.288468	-0.367794	-0.673473
C	1.288468	-0.367793	0.673473
H	2.178623	-0.106004	1.233684
H	2.178624	-0.106004	-1.233684
C	-0.024786	-0.488863	-1.360193
C	-0.024785	-0.488862	1.360194
C	-1.079386	0.790934	-0.768483
C	-1.079385	0.790935	0.768483
H	-2.066460	0.584537	-1.184659
H	-2.066460	0.584539	1.184660
H	-0.703080	1.721846	-1.192195
H	-0.703079	1.721847	1.192194
H	-0.552905	-1.404240	-1.085533
H	-0.552906	-1.404240	1.085535
H	0.047013	-0.437209	-2.446049
H	0.047014	-0.437208	2.446050

Point 12 Energy= -0.23409504172293E+03

C	1.286689	-0.364800	-0.672588
C	1.286689	-0.364800	0.672587
H	2.180446	-0.125735	1.237137
H	2.180445	-0.125735	-1.237137
C	-0.037835	-0.473453	-1.354552
C	-0.037835	-0.473452	1.354552
C	-1.065226	0.773726	-0.772962
C	-1.065225	0.773727	0.772962
H	-2.059597	0.582229	-1.180299
H	-2.059597	0.582230	1.180299
H	-0.697803	1.713275	-1.186849
H	-0.697802	1.713275	1.186848
H	-0.549962	-1.402046	-1.090473
H	-0.549962	-1.402046	1.090475
H	0.038071	-0.423029	-2.440569
H	0.038073	-0.423027	2.440569

Point 13 Energy= -0.23410226888182E+03

C	1.284228	-0.361500	-0.671889
C	1.284228	-0.361500	0.671889
H	2.181439	-0.147413	1.240864
H	2.181440	-0.147413	-1.240864
C	-0.050291	-0.458124	-1.349161
C	-0.050290	-0.458123	1.349161

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C	-1.051031	0.756439	-0.776558
C	-1.051031	0.756440	0.776558
H	-2.051476	0.578231	-1.176074
H	-2.051476	0.578233	1.176075
H	-0.690865	1.703374	-1.181072
H	-0.690864	1.703376	1.181071
H	-0.547974	-1.398429	-1.095636
H	-0.547974	-1.398429	1.095639
H	0.028625	-0.407042	-2.435217
H	0.028627	-0.407040	2.435218

Point 14 Energy= -0.23410818150749E+03

C	1.280884	-0.357751	-0.671337
C	1.280884	-0.357751	0.671336
H	2.181484	-0.172062	1.244804
H	2.181485	-0.172064	-1.244805
C	-0.061932	-0.443025	-1.344281
C	-0.061932	-0.443025	1.344281
C	-1.036823	0.739119	-0.778991
C	-1.036823	0.739120	0.778991
H	-2.042185	0.572644	-1.171867
H	-2.042185	0.572646	1.171867
H	-0.682231	1.692270	-1.174545
H	-0.682230	1.692271	1.174544
H	-0.546809	-1.393663	-1.101626
H	-0.546809	-1.393664	1.101627
H	0.018742	-0.388658	-2.430198
H	0.018743	-0.388657	2.430199

Point 15 Energy= -0.23411243439658E+03

C	1.276236	-0.353327	-0.670916
C	1.276236	-0.353327	0.670916
H	2.180299	-0.201551	1.248642
H	2.180299	-0.201551	-1.248643
C	-0.072254	-0.428447	-1.340575
C	-0.072254	-0.428447	1.340576
C	-1.022732	0.721900	-0.779713
C	-1.022732	0.721901	0.779713
H	-2.031801	0.565657	-1.167396
H	-2.031799	0.565657	1.167396
H	-0.671768	1.680059	-1.166635
H	-0.671766	1.680059	1.166635
H	-0.546114	-1.388288	-1.109984
H	-0.546114	-1.388287	1.109984
H	0.008845	-0.366577	-2.426067
H	0.008845	-0.366576	2.426068

Point 16 Ener gy= -0.234 11480328287E+03

C		-0.348132	-0.670598

1.269487

C	1.269487	-0.348131	0.670598
H	2.177875	-0.239736	1.250999
H	2.177874	-0.239735	-1.250999
C	-0.079755	-0.415137	-1.34045
C	-0.079754	-0.415137	1.340451
C	-1.009674	0.705468	-0.777862

Point boat Energy= -0.23411480328287E+03

C	1.2544336372	-0.3517921494	-0.6702613561
C	1.2544349919	-0.3517928006	0.6702585226
H	2.1781771378	-0.3312373300	1.2361610284
H	2.1781746393	-0.3312361291	-1.2361657089
C	-0.0742164491	-0.3767561584	-1.3778165455
C	-0.0742136643	-0.3767574969	1.3778163732
C	-1.0226101922	0.6810524614	-0.7750700615
C	-1.0226086256	0.6810517085	0.7750728337
H	-2.0323182257	0.5156552304	-1.1560660127
H	-2.0323158899	0.5156541074	1.1560706650
H	-0.7062198155	1.6610390631	-1.1361281176
H	-0.7062175192	1.6610379594	1.1361312023
H	-0.5265649961	-1.3682936625	-1.2617576500
H	-0.5265624458	-1.3682948883	1.2617574287
H	0.0406286829	-0.2074333292	-2.4489141359
H	0.0406336327	-0.2074357082	2.4489138960

Point hchair Energy= -0.23412452069069E+03

H	-0.2772136296	2.4202259961	0.1608833045
C	0.2609431885	1.4761340701	0.0409964258
C	-0.1257214107	-0.6580218158	1.2996407438
C	0.2630421938	-0.7182009729	-1.1815757930
C	-0.2609431885	-1.4761340701	0.0409964258
C	-0.2630421938	0.7182009729	-1.1815757930
C	0.1257214107	0.6580218158	1.2996407438
H	1.3570132507	-0.6971336657	-1.1508057587
H	-1.3133302512	-1.7429292167	-0.1088632517
H	-1.3570132507	0.6971336657	-1.1508057587
H	1.3133302512	1.7429292167	-0.1088632517
H	-0.2355940282	-1.1735918975	2.2481503810
H	-0.0250882426	-1.2368570710	-2.0984001960
H	0.2772136296	-2.4202259961	0.1608833045
H	0.0250882426	1.2368570710	-2.0984001960
H	0.2355940282	1.1735918975	2.2481503810

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C	-1.009674	0.705469	0.777862
H	-2.021175	0.558149	-1.162291
H	-2.021175	0.558150	1.162291
H	-0.660007	1.667433	-1.156332
H	-0.660005	1.667431	1.156331
H	-0.544576	-1.383709	-1.126213
H	-0.544577	-1.383705	1.126212
H	0.001541	-0.337524	-2.424795
H	0.001540	-0.337524	2.424796

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IRC of the 1+3 cycloaddition
SCS-MP2/*aug*-cc-pVTZ electronic energies in a.u.
Point -18 Energy= -0.27208088262240E+03

C	-0.184963	-0.727558	-1.415481
C	0.563539	0.395724	-1.312017
C	0.965822	-0.976234	0.556521
C	0.065192	-1.580697	-0.253549
H	-0.872976	-0.960411	-2.216265
H	-0.411547	-2.534090	-0.072994
C	1.414503	0.310898	-0.076259
H	1.309722	1.175296	0.580977
H	2.474477	0.244827	-0.352975
C	-1.459110	1.503585	0.577226
H	-0.897960	2.413795	0.409494
H	-2.218520	1.255995	-0.151409
C	-1.230731	0.724725	1.637996
H	-0.475341	0.972477	2.372506
H	-1.797225	-0.180794	1.805429
H	0.597368	1.213041	-2.018070
H	1.352405	-1.361960	1.488953

Point -17 Energy= -0.27208024098493E+03

C	-0.188378	-0.725315	-1.412642
C	0.552755	0.402765	-1.304312
C	0.954981	-0.968995	0.563957
C	0.061654	-1.578030	-0.251286
H	-0.872743	-0.960349	-2.215919
H	-0.411405	-2.533703	-0.073089
C	1.405429	0.317092	-0.069758
H	1.312429	1.183194	0.586192
H	2.463232	0.241309	-0.353138
C	-1.441688	1.491943	0.564797
H	-0.879835	2.401490	0.395997
H	-2.203716	1.246437	-0.161714
C	-1.213275	0.712963	1.625732
H	-0.457057	0.959651	2.359714
H	-1.782393	-0.190445	1.795252
H	0.584955	1.220939	-2.009466
H	1.339959	-1.353939	1.497392

Point -16 Energy= -0.27207951139365E+03

C	-0.191557	-0.723242	-1.409911
C	0.541693	0.409901	-1.296444
C	0.943851	-0.961629	0.571514
C	0.058333	-1.575472	-0.249216
H	-0.872135	-0.960503	-2.215749
H	-0.410911	-2.533474	-0.073438
C	1.396446	0.323188	-0.063349
H	1.316393	1.191143	0.591174
H	2.451777	0.236634	-0.354106
C	-1.424268	1.480407	0.552411
H	-0.862378	2.389772	0.383056
H	-2.188679	1.236817	-0.172134
C	-1.195810	0.701273	1.613554
H	-0.439446	0.947399	2.347501
H	-1.767323	-0.200175	1.784983
H	0.572205	1.228933	-2.000686
H	1.327164	-1.345791	1.505961

Point -15 Energy= -0.27207868612769E+03
C -0.194536 -0.721316 -1.407261

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C	0.530387	0.417133	-1.288418
C	0.932470	-0.954136	0.579184
C	0.055193	-1.572994	-0.247315
H	-0.871255	-0.960804	-2.215696
H	-0.410155	-2.533345	-0.073972
C	1.387593	0.329145	-0.057069
H	1.321340	1.198883	0.595793
H	2.439993	0.231009	-0.355698
C	-1.406853	1.468965	0.540062
H	-0.845477	2.378574	0.370588
H	-2.173483	1.227171	-0.182652
C	-1.178340	0.689649	1.601456
H	-0.422377	0.935638	2.335803
H	-1.752082	-0.209973	1.774672
H	0.559138	1.237054	-1.991740
H	1.314051	-1.337510	1.514694

Point -14 Energy= -0.27207775750867E+03

C	-0.197295	-0.719535	-1.404678
C	0.518817	0.424472	-1.280208
C	0.920810	-0.946492	0.586977
C	0.052249	-1.570583	-0.245593
H	-0.870096	-0.961235	-2.215715
H	-0.409145	-2.533268	-0.074679
C	1.378935	0.334944	-0.050947
H	1.327503	1.206536	0.600085
H	2.427989	0.224277	-0.358058
C	-1.389467	1.457603	0.527726
H	-0.829311	2.367988	0.358720
H	-2.158158	1.217531	-0.193215
C	-1.160886	0.678055	1.589437
H	-0.406043	0.924485	2.324707
H	-1.736705	-0.219785	1.764347
H	0.545786	1.245228	-1.982607
H	1.300629	-1.329102	1.523502

Point -13 Energy= -0.27207671784425E+03

C	-0.199838	-0.717892	-1.402142
C	0.506988	0.431918	-1.271799
C	0.908876	-0.938678	0.594888
C	0.049495	-1.568216	-0.244042
H	-0.868728	-0.961762	-2.215774
H	-0.407944	-2.533222	-0.075520
C	1.370529	0.340560	-0.045015
H	1.334742	1.213910	0.603938
H	2.415753	0.216507	-0.361130
C	-1.372120	1.446312	0.515395
H	-0.813799	2.357950	0.347381
H	-2.142924	1.207987	-0.203773
C	-1.143455	0.666480	1.577491
H	-0.390359	0.913864	2.314162
H	-1.721398	-0.229580	1.754128
H	0.532160	1.253522	-1.973341
H	1.286941	-1.320579	1.532462

Point -12 Energy= -0.27207555967311E+03

C	-0.202162	-0.716388	-1.399643
C	0.494894	0.439488	-1.263168
C	0.896654	-0.930674	0.602928
C	0.046928	-1.565882	-0.242671
H	-0.867159	-0.962355	-2.215817
H	-0.406573	-2.533136	-0.076487
C	1.362441	0.345954	-0.039313
H	1.343140	1.221039	0.607364

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H	2.403283	0.207671	-0.364933
C	-1.354829	1.435086	0.503045
H	-0.799065	2.348504	0.336660
H	-2.127781	1.198600	-0.214234
C	-1.126060	0.654898	1.565626
H	-0.375459	0.903850	2.304214
H	-1.706168	-0.239253	1.744058
H	0.518309	1.261817	-1.963881
H	1.272983	-1.311926	1.541435

Point -11 Energy= -0.27207427622216E+03

C	-0.204255	-0.715030	-1.397163
C	0.482520	0.447183	-1.254276
C	0.884123	-0.922443	0.611090
C	0.044555	-1.563569	-0.241493
H	-0.865437	-0.963016	-2.215843
H	-0.405077	-2.533030	-0.077558
C	1.354745	0.351101	-0.033877
H	1.352623	1.227756	0.610256
H	2.390658	0.197794	-0.369468
C	-1.337604	1.423918	0.490664
H	-0.785153	2.339708	0.326594
H	-2.112966	1.189453	-0.224574
C	-1.108707	0.643292	1.553843
H	-0.361381	0.894489	2.294920
H	-1.691237	-0.248801	1.734265
H	0.504275	1.270196	-1.954338
H	1.258850	-1.303204	1.550511

Point -10 Energy= -0.27207286208338E+03

C	-0.206113	-0.713838	-1.394699
C	0.469852	0.455024	-1.245092
C	0.871266	-0.913954	0.619392
C	0.042373	-1.561276	-0.240527
H	-0.863553	-0.963729	-2.215786
H	-0.403460	-2.532829	-0.078745
C	1.347521	0.355956	-0.028757
H	1.363184	1.234104	0.612642
H	2.377870	0.186930	-0.374692
C	-1.320464	1.412816	0.478219
H	-0.772217	2.331595	0.317294
H	-2.098517	1.180670	-0.234620
C	-1.091403	0.631631	1.542158
H	-0.348294	0.885857	2.286324
H	-1.676655	-0.258034	1.724834
H	0.490149	1.278457	-1.944637
H	1.244563	-1.294391	1.559464

Point -9 Energy= -0.27207131433526E+03

C	-0.207726	-0.712835	-1.392232
C	0.456874	0.463003	-1.235557
C	0.858048	-0.905158	0.627814
C	0.040385	-1.558992	-0.239806
H	-0.861557	-0.964528	-2.215682
H	-0.401768	-2.532590	-0.080052
H	0.476055	1.28669 3	-1.934993
H	1.230316	-1.285633	1.568398

Point -8 Energy= -0.27206963431645E+03

C	-0.209097	-0.712066	-1.389760
C	0.443574	0.471150	-1.225634
C	0.844455	-0.896013	0.636377
C	0.038577	-1.556730	-0.239367
H	-0.859400	-0.965419	-2.215457
H	-0.399976	-2.532235	-0.081523
C	1.334860	0.364675	-0.019630
H	1.387038	1.245197	0.615652
H	2.352301	0.162661	-0.387007
C	-1.286471	1.390834	0.453028
H	-0.749855	2.317900	0.301479
H	-2.071752	1.164752	-0.253450
C	-1.056939	0.608045	1.519153
H	-0.325674	0.871287	2.271700
H	-1.649517	-0.275231	1.707744
H	0.462189	1.294549	-1.925321
H	1.216201	-1.276928	1.576910

Point -7 Energy= -0.27206783052931E+03

C	-0.210225	-0.711578	-1.387262
C	0.429947	0.479443	-1.215249
C	0.830460	-0.886456	0.645044
C	0.036933	-1.554485	-0.239262
H	-0.857148	-0.966480	-2.215198
H	-0.398137	-2.531890	-0.083182
C	1.329614	0.368481	-0.015706
H	1.399978	1.249789	0.616236
H	2.339822	0.149605	-0.393906
C	-1.269639	1.379998	0.440196
H	-0.740851	2.312608	0.295307
H	-2.059979	1.157964	-0.261903
C	-1.039767	0.596049	1.507899
H	-0.316577	0.865672	2.265971
H	-1.637489	-0.282883	1.700467
H	0.448821	1.302162	-1.916013
H	1.202606	-1.268537	1.585157

Point -6 Energy= -0.27206592305149E+03

C	-0.211140	-0.711443	-1.384738
C	0.416012	0.487928	-1.204385
C	0.816080	-0.876459	0.653847
C	0.035414	-1.552286	-0.239548
H	-0.854719	-0.967732	-2.214807
H	-0.396206	-2.531439	-0.085108
C	1.325222	0.371865	-0.012275
H	1.413286	1.253905	0.616395
H	2.327686	0.136320	-0.401046
C	-1.252952	1.369324	0.427111
H	-0.733717	2.308455	0.290577
H	-2.049450	1.152271	-0.269258
C	-1.022630	0.583843	1.496903

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C	1.340860	0.360498	-0.023988
H	1.374688	1.239884	0.614408
H	2.365078	0.175164	-0.380577
C	-1.303412	1.401781	0.465691
H	-0.760369	2.324311	0.308868
H	-2.084759	1.172371	-0.244342
C	-1.074147	0.619897	1.530581
H	-0.336303	0.878086	2.278564
H	-1.662716	-0.266952	1.715952
H	-0.852238	-0.969290	-2.214442
H	-0.394279	-2.531110	-0.087318
C	1.321731	0.374850	-0.009331
H	1.426566	1.257195	0.615951
H	2.316342	0.123106	-0.408308
C	-1.236414	1.358873	0.413721
H	-0.728591	2.305733	0.287475
H	-2.040814	1.147778	-0.275525
C	-1.005507	0.571395	1.486232
H	-0.304277	0.858663	2.258321
H	-1.617777	-0.294937	1.689390
H	0.424915	1.315275	-1.898660
H	1.177996	-1.253037	1.599259

Point -4 Energy= -0.27206197965370E+03

C	-0.212472	-0.712506	-1.379565
C	0.387431	0.505432	-1.181107
C	0.786339	-0.854999	0.671736
C	0.032542	-1.548100	-0.241525
H	-0.849601	-0.971164	-2.213944
H	-0.392303	-2.530719	-0.089903
C	1.319187	0.377403	-0.006909
H	1.439512	1.260156	0.615337
H	2.305757	0.110383	-0.415370
C	-1.220089	1.348737	0.399926
H	-0.725796	2.304249	0.286108
H	-2.033806	1.144745	-0.280183
C	-0.988411	0.558631	1.476018
H	-0.301570	0.857484	2.256542
H	-1.610517	-0.298827	1.685897
H	0.415067	1.320341	-1.890811
H	1.167605	-1.246110	1.604576

Point -3 Energy= -0.27206011849723E+03

C	-0.213018	-0.713861	-1.376913
C	0.372994	0.514511	-1.168742
C	0.771197	-0.843520	0.680832
C	0.031038	-1.546187	-0.243324
H	-0.847011	-0.973271	-2.213655
H	-0.390368	-2.530610	-0.092631
C	1.317492	0.379566	-0.004957
H	1.451707	1.262267	0.614262
H	2.296518	0.098539	-0.422078
C	-1.204005	1.339031	0.385661
H	-0.725052	2.304152	0.286527
H	-2.029043	1.142933	-0.283495
H	-0.309400	0.861385	2.261419
H	-1.626713	-0.289418	1.694261
H	0.436273	1.308965	-1.906923
H	1.189679	-1.260442	1.592491

Point -5 Energy= -0.27206395041523E+03

C	-0.211868	-0.711732	-1.382164
C	0.401817	0.496573	-1.192983
C	0.801342	-0.865964	0.662728
C	0.033971	-1.550139	-0.240292
H	-2.026210	1.142990	-0.284532
C	-0.954192	0.531988	1.457299
H	-0.303233	0.860118	2.256927
H	-1.602536	-0.301902	1.683344
H	0.399891	1.328550	-1.877217
H	1.151264	-1.233916	1.612746

Point -1 Energy= -0.27205741631347E+03

C	-0.214267	-0.718027	-1.371685
C	0.344260	0.533233	-1.143096
C	0.740913	-0.819505	0.699272
C	0.027612	-1.542927	-0.248209
H	-0.842805	-0.977663	-2.212689
H	-0.387540	-2.530284	-0.098093
C	1.316543	0.382933	-0.002281
H	1.469835	1.265827	0.612971
H	2.283275	0.081234	-0.431933
C	-1.172777	1.321134	0.355627
H	-0.728061	2.305668	0.289947
H	-2.024439	1.142959	-0.285179
C	-0.937340	0.518203	1.449183
H	-0.304463	0.861035	2.257470
H	-1.600700	-0.302156	1.683002
H	0.396714	1.329656	-1.873803
H	1.147566	-1.231034	1.613740

Point TS Energy= -0.27205701477687E+03

C	-0.2147725414	-0.7206767234	-1.3692818855
C	0.3303785133	0.5427639526	-1.1301447272
C	0.7262264773	-0.8072277498	0.7084830542
C	0.0259551473	-1.5416494496	-0.2511540781
H	-0.8384950624	-0.9820291794	-2.2133987862
H	-0.3841621203	-2.5314768401	-0.1031209898
C	1.3171418262	0.3836292957	-0.0018989946
H	1.4852031276	1.2664864834	0.6101461213
H	2.2749036438	0.0672361702	-0.4404087180
C	-1.1585343135	1.3135384427	0.3407403673
H	-0.7352553009	2.3090200852	0.2970262684
H	-2.0240810357	1.1444216816	-0.2841866209
C	-0.9214011454	0.5048243951	1.4421724076
H	-0.3124906801	0.8672323742	2.2606760713
H	-1.6003392959	-0.3006983761	1.6840016878
H	0.3915147903	1.3330528342	-1.8672169016
H	1.1415590972	-1.2248827436	1.6165759306

Point 1 Energy= -0.27205747430117E+03

C	-0.215428	-0.723486	-1.366963

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C -0.971329 0.545520 1.466388
H -0.301002 0.857989 2.256140
H -1.605494 -0.301522 1.683796
H 0.406920 1.324810 -1.884243
H 1.159043 -1.240223 1.609206
Point -2 Energy= -0.27205852652693E+03
C -0.213681 -0.715684 -1.374254
C 0.358753 0.523598 -1.156182
C 0.756191 -0.831818 0.689834
C 0.029329 -1.544440 -0.245528
H -0.844212 -0.976410 -2.213174
H -0.388490 -2.530608 -0.096423
C 1.316515 0.381658 -0.003210
H 1.463640 1.264586 0.613394
H 2.287732 0.087204 -0.428508
C -1.188099 1.329701 0.370850
H -0.726941 2.305118 0.288900
C -0.216398 -0.726436 -1.364662
C 0.302663 0.562532 -1.103515
C 0.696841 -0.781765 0.727357
C 0.022022 -1.539537 -0.257254
H -0.831913 -0.988368 -2.214884
H -0.378831 -2.533567 -0.110391
C 1.319239 0.384709 -0.001558
H 1.504698 1.267403 0.606622
H 2.264928 0.050284 -0.450708
C -1.129966 1.298977 0.309079
H -0.747005 2.312594 0.307807
H -2.024626 1.147408 -0.280210
C -0.888808 0.476537 1.429205
H -0.325769 0.876017 2.264359
H -1.601337 -0.296169 1.685874
H 0.386130 1.336149 -1.857725
H 1.134532 -1.216174 1.618423
Point 3 Energy= -0.27206171277163E+03
C -0.217687 -0.729344 -1.362429
C 0.289115 0.572375 -1.090164
C 0.682422 -0.768952 0.736663
C 0.019622 -1.538656 -0.260182
H -0.828331 -0.992292 -2.215707
H -0.376012 -2.534868 -0.114783
C 1.320212 0.385729 -0.001018
H 1.513245 1.268722 0.605750
H 2.260106 0.043382 -0.454737
C -1.115245 1.291660 0.292287
C 0.316694 0.552423 -1.117067
C 0.711717 -0.794753 0.717726
C 0.024148 -1.540531 -0.254184
H -0.833857 -0.986695 -2.214430
H -0.380444 -2.533000 -0.108432
C 1.318101 0.384127 -0.001740
H 1.500290 1.266860 0.607172
H 2.266949 0.053796 -0.448565
C -1.144531 1.306326 0.325473
H -0.743418 2.312129 0.304844
H -2.024458 1.146316 -0.282171
C -0.905509 0.491168 1.435681
H -0.321680 0.873840 2.263729
H -1.600864 -0.298301 1.685331
H 0.386949 1.336237 -1.860634
H 1.136108 -1.218677 1.619044
Point 2 Energy= -0.27205900657970E+03
H 1.528975 1.269995 0.603298
H 2.251823 0.031378 -0.461767
C -1.086183 1.277589 0.258340
H -0.765296 2.312524 0.324870
H -2.024606 1.151977 -0.269363
C -0.838070 0.431430 1.410770
H -0.347639 0.888151 2.264799
H -1.603353 -0.284656 1.687265
H 0.379208 1.339627 -1.841108
H 1.124191 -1.201049 1.619181
Point 6 Energy= -0.27207674096751E+03
C -0.222160 -0.737355 -1.356235
C 0.248463 0.602679 -1.049669
C 0.639192 -0.729856 0.765183
C 0.012131 -1.536374 -0.268007
H -0.815274 -1.002623 -2.221237
H -0.364278 -2.540697 -0.126452
C 1.323162 0.387806 -0.000128
H 1.536632 1.270461 0.601992
H 2.247511 0.025615 -0.465071
C -1.071604 1.270561 0.241322
H -0.770414 2.310707 0.329912
H -2.023284 1.152152 -0.266023
C -0.821123 0.416326 1.404750
H -0.354189 0.891221 2.263189
H -1.602979 -0.281243 1.686195
H 0.376928 1.340703 -1.835612
H 1.120766 -1.196071 1.619360

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H -0.753491 2.313366 0.313634
H -2.025046 1.149626 -0.276520
C -0.871847 0.461578 1.422819
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H -1.602292 -0.292126 1.687080
H 0.383421 1.337521 -1.851678
H 1.130608 -1.210674 1.618851
Point 4 Energy= -0.27206562011189E+03
C -0.219054 -0.732240 -1.360269
C 0.275570 0.582425 -1.076637
C 0.668000 -0.755908 0.746113
C 0.017171 -1.537854 -0.263058
H -0.824498 -0.995794 -2.217250
H -0.372682 -2.536659 -0.118663
C 1.321272 0.386485 -0.000691
H 1.521173 1.269154 0.604361
H 2.256020 0.037232 -0.458373
C -1.100687 1.284579 0.275370
H -0.759504 2.313469 0.319392
H -2.025350 1.151011 -0.273094
C -0.854957 0.446547 1.416731
H -0.340508 0.884536 2.265536
H -1.603232 -0.288568 1.687547
H 0.381306 1.338970 -1.846764
H 1.127571 -1.206080 1.619483
Point 5 Energy= -0.27207067824846E+03
C -0.220552 -0.734949 -1.358221
C 0.262033 0.592577 -1.063155
C 0.653617 -0.742872 0.755668
C 0.014663 -1.537123 -0.265695
H -0.820098 -0.999230 -2.218995
H -0.368751 -2.538492 -0.122586
C 1.322299 0.387135 -0.000435
H -1.598642 -0.276233 1.680688
H 0.370509 1.343120 -1.822943
H 1.111763 -1.184844 1.620030
Point 9 Energy= -0.27209852394202E+03
C -0.227710 -0.741869 -1.350461
C 0.207441 0.632452 -1.009840
C 0.595688 -0.691619 0.793487
C 0.004436 -1.533578 -0.272190
H -0.797139 -1.011566 -2.229953
H -0.346618 -2.548012 -0.137382
C 1.323858 0.390136 0.001433
H 1.560120 1.272210 0.598219
H 2.231313 0.007599 -0.474811
C -1.027074 1.248415 0.190934
Point 7 Energy= -0.27208358547396E+03
C -0.223885 -0.739362 -1.354311
C 0.234836 0.612737 -1.036273
C 0.624729 -0.716947 0.774698
C 0.009583 -1.535578 -0.269900
H -0.809848 -1.005840 -2.223782
H -0.359117 -2.542997 -0.130239
C 1.323763 0.388498 0.000251
H 1.544344 1.271087 0.600792
H 2.242746 0.019825 -0.468296
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H -2.020607 1.151388 -0.263128
C -0.804123 0.401264 1.398575
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H -1.601399 -0.278273 1.684004
H 0.374091 1.341692 -1.829473
H 1.116625 -1.190634 1.619442
Point 8 Energy= -0.27209094322331E+03
C -0.225728 -0.740884 -1.352400
C 0.221150 0.622670 -1.022975
C 0.610213 -0.704181 0.784137
C 0.007025 -1.534663 -0.271309
H -0.803829 -1.008847 -2.226708
H -0.353258 -2.545472 -0.133895
C 1.324017 0.389268 0.000761
H 1.552144 1.271635 0.599514
H 2.237407 0.013851 -0.471534
C -1.042083 1.256049 0.207560
H -0.777448 2.303593 0.337659
H -2.016705 1.149519 -0.261120
C -0.787053 0.386299 1.392120
H -0.364334 0.894717 2.256485
C -0.004023 -1.528524 -0.271374
H -0.772115 -1.017353 -2.241426
H -0.321096 -2.555502 -0.146538
C 1.320447 0.393585 0.004699
H 1.585737 1.273912 0.593953
H 2.207190 -0.013646 -0.485217
C -0.981112 1.223289 0.142396
H -0.773631 2.276021 0.339957
H -1.987039 1.129810 -0.265082
C -0.718482 0.327620 1.362256
H -0.366863 0.888787 2.229311
H -1.573565 -0.280292 1.655412
H 0.345748 1.354868 -1.791059
H 1.082134 -1.156490 1.629298

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H	-0.778893	2.298332	0.340010
H	-2.011331	1.146466	-0.260158
C	-0.769929	0.371450	1.385320
H	-0.367382	0.894922	2.251389
H	-1.594454	-0.275246	1.676150
H	0.365964	1.344990	-1.815792
H	1.105915	-1.178528	1.621127

Point 10 Energy= -0.27210602435037E+03

C	-0.229858	-0.742282	-1.348425
C	0.193765	0.642051	-0.996920
C	0.581218	-0.679309	0.802714
C	0.001779	-1.532252	-0.272521
H	-0.789706	-1.013940	-2.233502
H	-0.339129	-2.550579	-0.140671
C	1.323238	0.391128	0.002295
H	1.568327	1.272782	0.596872
H	2.224339	0.000982	-0.478169
C	-1.011895	1.240453	0.174525
H	-0.778758	2.291960	0.341173
H	-2.004589	1.142193	-0.260423
C	-0.752768	0.356731	1.378113
H	-0.368842	0.893989	2.245147
H	-1.588885	-0.275515	1.670430
H	0.360368	1.347497	-1.808086
H	1.099052	-1.171705	1.622953

Point 11 Energy= -0.27211312497632E+03

C	-0.232222	-0.742078	-1.346209
C	0.180212	0.651445	-0.984300
C	0.566902	-0.667317	0.811796
C	-0.001008	-1.530606	-0.272270
H	-0.781425	-1.015899	-2.237333
H	-0.330682	-2.553100	-0.143734
C	1.322114	0.392268	0.003373
H	1.576831	1.273348	0.595457
H	2.216350	-0.006071	-0.481627
C	-0.996566	1.232105	0.158344
H	-0.777016	2.284543	0.341172
H	-1.996437	1.136657	-0.262035
C	-0.735605	0.342130	1.370449
H	-0.368680	0.891961	2.237804
H	-1.581876	-0.277155	1.663510
H	0.353640	1.350741	-1.799820
H	1.091121	-1.164352	1.625625

Point 12 Energy= -0.27211948236329E+03

C	-0.234889	-0.741183	-1.343696
C	0.166916	0.660617	-0.972095
C	0.552898	-0.655729	0.820711
H	-0.757796	2.241679	0.330933
H	-1.951570	1.095796	-0.288097
C	-0.670137	0.283149	1.332038
H	-0.356356	0.872603	2.195563
H	-1.540704	-0.305417	1.620294
H	0.317524	1.374583	-1.764804

Point 13 Energy= -0.27212472298455E+03

C	-0.238034	-0.739433	-1.340688
C	0.154113	0.669542	-0.960509
C	0.539477	-0.644696	0.829424
C	-0.007452	-1.525805	-0.269685
H	-0.761483	-1.018156	-2.245778
H	-0.310063	-2.557668	-0.149032
C	1.318192	0.395128	0.006318
H	1.595215	1.274448	0.592306
H	2.196646	-0.021866	-0.488982
C	-0.965599	1.213842	0.126677
H	-0.768691	2.266412	0.337704
H	-1.976297	1.121439	-0.269823
C	-0.701490	0.313132	1.353403
H	-0.363516	0.884608	2.219656
H	-1.563833	-0.285220	1.645981
H	0.336696	1.360058	-1.781927
H	1.072167	-1.148177	1.634177

Point 14 Energy= -0.27212844998981E+03

C	-0.242074	-0.736393	-1.336746
C	0.142378	0.678183	-0.949992
C	0.527295	-0.634531	0.837866
C	-0.011721	-1.521987	-0.266803
H	-0.749100	-1.017940	-2.250259
H	-0.297144	-2.559280	-0.151024
C	1.315343	0.396981	0.008291
H	1.605622	1.274964	0.590445
H	2.184467	-0.030893	-0.492989
C	-0.950208	1.203389	0.111186
H	-0.762464	2.255281	0.334486
H	-1.964344	1.110976	-0.276781
C	-0.684878	0.298509	1.343591
H	-0.358997	0.879309	2.208498
H	-1.552776	-0.292627	1.634863
H	0.326646	1.366582	-1.772709
H	1.061503	-1.139557	1.640539

Point 15 Energy= -0.27213031405902E+03

C	-0.248528	-0.730547	-1.330419
C	0.134229	0.686394	-0.942029
C	0.519098	-0.626154	0.845602
C	-0.018349	-1.515543	-0.261290
H	-0.736642	-1.015043	-2.253135
H	-0.284056	-2.558534	-0.150970
C	1.312809	0.399290	0.010533
H	1.617837	1.275523	0.588225
H	2.171728	-0.040378	-0.497209
C	-0.936255	1.190712	0.095977

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H 1.052363 -1.131494 1.648359

Point Pr Energy= -0.27213065058418E+03

C	-0.2622088335	-0.7175468236	-1.3176381325
C	0.1398557615	0.6948596573	-0.9381734988
C	0.5250378134	-0.6187510187	0.8509066590
C	-0.0321079286	-1.5022744704	-0.2488734765
H	-0.7618658760	-0.9978623543	-2.2353022109
H	-0.3092198493	-2.5415496839	-0.1328677364
C	1.3192550021	0.4025339093	0.0115253538
H	1.6344117657	1.2773219839	0.5859759846
H	2.1718135919	-0.0446472687	-0.5003646431
C	-0.9312449951	1.1818723762	0.0877354891
H	-0.7703907995	2.2334373889	0.3323007372
H	-1.9423326513	1.0750597274	-0.3042405810
C	-0.6649432109	0.2736865847	1.3246447263
H	-0.3702223247	0.8687175688	2.1909893090
H	-1.5317539271	-0.3251628238	1.6028011541
H	0.3216225830	1.3822502408	-1.7616446634
H	1.0568947618	-1.1252949033	1.6535219031

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SCS-MP2/aug-cc-pVTZ energies of the stationary points

Without scaling vibrational frequencies.

	E	**E0**	**H**	**G**
ethene (**1**)	-78.410423	-78.359229	-78.355234	-78.380104
1,3-butadiene (**2**) strans	-155.641144	-155.555942	-155.550287	-155.581822
1,3-butadiene (**2**) scis skw	-155.636646	-155.551343	-155.545710	-155.577323
1,3-butadiene (**2**) scis flat	-155.635267	-155.550340	-155.545328	-155.576417
cyclopentadiene (**3**)	-193.670562	-193.577770	-193.572659	-193.603725
1 + **2**	-234.051567	-233.915171	-233.905521	-233.961926
TS (**1** + **2**)	-234.018485	-233.878373	-233.870975	-233.907932
cyclohexene (**4**) boat	-234.115996	-233.969069	-233.962287	-233.998990
cyclohexene (**4**) h-chair	-234.124521	-233.977129	-233.970685	-234.005098
1 + 3	-272.080984	-271.936999	-271.927893	-271.983829
TS (**1** + **3**)	-272.057015	-271.909513	-271.902414	-271.938974
norbornene (**5**)	-272.130651	-271.976990	-271.970810	-272.005536

After scaling vibrational frequencies (scaling factor of 0.9586).

	E	**E0**	**H**	**G**
ethene (**1**)	-78.410423	-78.361348	-78.357317	-78.382234
1,3-butadiene (**2**) strans	-155.641144	-155.559469	-155.553690	-155.585431
1,3-butadiene (**2**) scis skw	-155.636646	-155.554875	-155.549119	-155.580936
1,3-butadiene (**2**) scis flat	-155.635267	-155.553857	-155.548731	-155.579988
cyclopentadiene (**3**)	-193.670562	-193.581612	-193.576357	-193.607626
1 + **2**	-234.051567	-233.920817	-233.911007	-233.967665
TS (**1** + **2**)	-234.018485	-233.884174	-233.876539	-233.913891
cyclohexene (**4**) boat	-234.115996	-233.975152	-233.968175	-234.005203
cyclohexene (**4**) h-chair	-234.124521	-233.983232	-233.976584	-234.011317
1 + 3	-272.080984	-271.942959	-271.933673	-271.989859
TS (**1** + **3**)	-272.057015	-271.915619	-271.908269	-271.945226
norbornene (**5**)	-272.130651	-271.983352	-271.976939	-272.012005

Energies in a.u.

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SCS-MP2/aug-cc-pVTZ 1+2 IRC relative energies

r	ΔE (kJ/mol)	ΔE(kcal/mol)	E(au)	E reactants
2.874	22.93	5.48	-234.042834	-234.051567
2.834	25.40	6.07	-234.041892	
2.794	28.22	6.75	-234.040817	
2.753	31.43	7.51	-234.039597	
2.713	35.04	8.37	-234.038222	
2.672	39.08	9.34	-234.036682	
2.630	43.56	10.41	-234.034974	
2.589	48.49	11.59	-234.033099	
2.546	53.82	12.86	-234.031066	
2.504	59.52	14.23	-234.028898	
2.460	65.46	15.64	-234.026636	
2.417	71.45	17.08	-234.024352	
2.373	77.18	18.45	-234.022170	
2.329	82.15	19.63	-234.020277	
2.284	85.64	20.47	-234.018950	
2.243	86.86	20.76	-234.018485	
2.203	85.37	20.40	-234.019052	
2.158	80.45	19.23	-234.020924	
2.114	71.73	17.14	-234.024247	
2.070	59.13	14.13	-234.029044	
2.026	42.88	10.25	-234.035233	
1.982	23.52	5.62	-234.042609	
1.937	1.79	0.43	-234.050886	
1.893	-21.49	-5.14	-234.059753	
1.849	-45.52	-10.88	-234.068903	
1.805	-69.49	-16.61	-234.078036	
1.761	-92.64	-22.14	-234.086853	
1.717	-114.14	-27.28	-234.095042	
1.675	-133.12	-31.82	-234.102269	
1.633	-148.64	-35.53	-234.108182	
1.594	-159.81	-38.19	-234.112434	
1.561	-166.03	-39.68	-234.114803	
1.543	-166.03	-39.68	-234.114803	
1.531	-191.54	-45.78	-234.124521	

Highlighted point corresponds to TS

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SCS-MP2/aug-cc-pVTZ 1+3 IRC relative energies

r	ΔE (kJ/mol)	ΔE(kcal/mol)	E(au)	E reactants
2.981	0.27	0.06	-272.080883	
2.942	1.95	0.47	-272.080241	-272.080984
2.903	3.87	0.92	-272.079511	
2.864	6.03	1.44	-272.078686	
2.824	8.47	2.02	-272.077758	
2.785	11.20	2.68	-272.076718	
2.744	14.24	3.40	-272.075560	
2.704	17.61	4.21	-272.074276	
2.663	21.33	5.10	-272.072862	
2.622	25.39	6.07	-272.071314	
2.580	29.80	7.12	-272.069634	
2.538	34.54	8.25	-272.067831	
2.495	39.54	9.45	-272.065923	
2.451	44.72	10.69	-272.063950	
2.407	49.90	11.93	-272.061980	
2.363	54.78	13.09	-272.060118	
2.318	58.96	14.09	-272.058527	
2.273	61.88	14.79	-272.057416	
2.230	62.93	15.04	-272.057015	
2.187	61.73	14.75	-272.057474	
2.142	57.70	13.79	-272.059007	
2.098	50.60	12.09	-272.061713	
2.053	40.34	9.64	-272.065620	
2.008	27.06	6.47	-272.070678	
1.963	11.14	2.66	-272.076741	
1.919	-6.83	-1.63	-272.083585	
1.874	-26.15	-6.25	-272.090943	
1.829	-46.05	-11.01	-272.098524	
1.784	-65.74	-15.71	-272.106024	
1.740	-84.39	-20.17	-272.113125	
1.696	-101.08	-24.16	-272.119482	
1.653	-114.84	-27.45	-272.124723	
1.611	-124.62	-29.79	-272.128450	
1.574	-129.52	-30.95	-272.130314	
1.561	-130.40	-31.17	-272.130651	

Highlighted point corresponds to TS

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SCS-MP2/aug-cc-pVTZ 1+2 IRC relative energies including CC

r	ΔE (kJ/mol)	ΔE (kcal/mol)	E (a.u.)	E reactants	CC (a.u.)	CC (kcal/mol)	CC (kJ/mol)
2.874	27.65	6.61	-234.041035	-234.051567	0.00179850	1.13	4.72
2.834	30.34	7.25	-234.040012		0.00187990	1.18	4.94
2.794	33.38	7.98	-234.038852		0.00196508	1.23	5.16
2.753	36.82	8.80	-234.037543		0.00205404	1.29	5.39
2.713	40.67	9.72	-234.036075		0.00214694	1.35	5.64
2.672	44.97	10.75	-234.034438		0.00224383	1.41	5.89
2.630	49.72	11.88	-234.032629		0.00234502	1.47	6.16
2.589	54.92	13.13	-234.030649		0.00245058	1.54	6.43
2.546	60.55	14.47	-234.028505		0.00256102	1.61	6.72
2.504	66.54	15.90	-234.026222		0.00267623	1.68	7.03
2.460	72.80	17.40	-234.023839		0.00279684	1.76	7.34
2.417	79.12	18.91	-234.021430		0.00292228	1.83	7.67
2.373	85.20	20.36	-234.019116		0.00305337	1.92	8.02
2.329	90.52	21.64	-234.017089		0.00318791	2.00	8.37
2.284	94.39	22.56	-234.015617		0.00333245	2.09	8.75
2.243	95.95	22.93	-234.015021		0.00346441	2.17	9.10
2.203	94.89	22.68	-234.015426		0.00362681	2.28	9.52
2.158	90.40	21.61	-234.017134		0.00378988	2.38	9.95
2.114	82.11	19.63	-234.020292		0.00395475	2.48	10.38
2.070	69.97	16.72	-234.024917		0.00412673	2.59	10.83
2.026	54.19	12.95	-234.030928		0.00430468	2.70	11.30
1.982	35.31	8.44	-234.038119		0.00448986	2.82	11.79
1.937	14.08	3.37	-234.046203		0.00468330	2.94	12.30
1.893	-8.66	-2.07	-234.054866		0.00488683	3.07	12.83
1.849	-32.12	-7.68	-234.063801		0.00510235	3.20	13.40
1.805	-55.50	-13.26	-234.072704		0.00533162	3.35	14.00
1.761	-78.00	-18.64	-234.081277		0.00557605	3.50	14.64
1.717	-98.82	-23.62	-234.089205		0.00583640	3.66	15.32
1.675	-117.07	-27.98	-234.096157		0.00611235	3.84	16.05
1.633	-131.83	-31.51	-234.101780		0.00640162	4.02	16.81
1.594	-142.23	-33.99	-234.105738		0.00669616	4.20	17.58
1.561	-147.74	-35.31	-234.107838		0.00696519	4.37	18.29
1.543	-150.60	-35.99	-234.108927		0.00706893	4.44	18.56
1.531	-172.95	-41.34	-234.117441		0.00707922	4.44	18.59

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SCS-MP2/aug-cc-pVTZ 1+3 IRC relative energies including CC

r	ΔE (kJ/mol)	ΔE (kcal/mol)	E (a.u.)	E reactants	CC (a.u.)	CC (kcal/mol)	CC (kJ/mol)
2.981	5.62	1.34	-272.078843	-272.080984	0.00203932	1.28	5.35
2.942	7.52	1.80	-272.078119		0.00212243	1.33	5.57
2.903	9.67	2.31	-272.077302		0.00220940	1.39	5.80
2.864	12.07	2.89	-272.076386		0.00230052	1.44	6.04
2.824	14.76	3.53	-272.075362		0.00239584	1.50	6.29
2.785	17.75	4.24	-272.074222		0.00249562	1.57	6.55
2.744	21.07	5.04	-272.072960		0.00259986	1.63	6.83
2.704	24.72	5.91	-272.071567		0.00270880	1.70	7.11
2.663	28.74	6.87	-272.070040		0.00282235	1.77	7.41
2.622	33.11	7.91	-272.068374		0.00294076	1.85	7.72
2.580	37.84	9.04	-272.066571		0.00306374	1.92	8.04
2.538	42.92	10.26	-272.064639		0.00319163	2.00	8.38
2.495	48.27	11.54	-272.062599		0.00332383	2.09	8.73
2.451	53.81	12.86	-272.060490		0.00346087	2.17	9.09
2.407	59.35	14.19	-272.058378		0.00360170	2.26	9.46
2.363	64.62	15.44	-272.056371		0.00374719	2.35	9.84
2.318	69.19	16.54	-272.054631		0.00389575	2.44	10.23
2.273	72.51	17.33	-272.053368		0.00404856	2.54	10.63
2.230	73.95	17.67	-272.052818		0.00419666	2.63	11.02
2.187	73.14	17.48	-272.053126		0.00434840	2.73	11.42
2.142	69.55	16.62	-272.054493		0.00451338	2.83	11.85
2.098	62.89	15.03	-272.057030		0.00468298	2.94	12.30
2.053	53.10	12.69	-272.060761		0.00485921	3.05	12.76
2.008	40.30	9.63	-272.065637		0.00504135	3.16	13.24
1.963	24.88	5.95	-272.071509		0.00523226	3.28	13.74
1.919	7.43	1.78	-272.078153		0.00543269	3.41	14.26
1.874	-11.33	-2.71	-272.085298		0.00564521	3.54	14.82
1.829	-30.63	-7.32	-272.092652		0.00587161	3.68	15.42
1.784	-49.69	-11.88	-272.099910		0.00611401	3.84	16.05
1.740	-67.65	-16.17	-272.106751		0.00637412	4.00	16.74
1.696	-83.61	-19.98	-272.112829		0.00665312	4.17	17.47
1.653	-96.59	-23.08	-272.117772		0.00695122	4.36	18.25
1.611	-105.54	-25.23	-272.121184		0.00726583	4.56	19.08
1.574	-109.62	-26.20	-272.122737		0.00757677	4.75	19.89
1.561	-110.13	-26.32	-272.122930		0.00772025	4.84	20.27

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SCS-MP2/aug-cc-pVTZ 1+2 IRC RHF energies

ethene:	-78.064611	**butadiene:**	-154.978749			
r	**complex**	**butadiene-fo**	**ethene-fo**	**butadiene**	**ethene**	**CC**
2.874	-233.018560	-154.971069	-78.064635	-154.970943	-78.064531	0.000230
2.834	-233.016683	-154.970836	-78.064615	-154.970706	-78.064507	0.000239
2.794	-233.014599	-154.970525	-78.064582	-154.970390	-78.064470	0.000248
2.753	-233.012291	-154.970116	-78.064534	-154.969977	-78.064416	0.000257
2.713	-233.009737	-154.969586	-78.064459	-154.969441	-78.064336	0.000267
2.672	-233.006919	-154.968909	-78.064349	-154.968760	-78.064221	0.000278
2.630	-233.003814	-154.968053	-78.064182	-154.967898	-78.064048	0.000289
2.589	-233.000405	-154.966980	-78.063935	-154.966819	-78.063795	0.000301
2.546	-232.996669	-154.965636	-78.063562	-154.965469	-78.063416	0.000313
2.504	-232.992594	-154.963951	-78.062999	-154.963777	-78.062847	0.000325
2.460	-232.988169	-154.961817	-78.062142	-154.961637	-78.061985	0.000338
2.417	-232.983448	-154.959119	-78.060879	-154.958933	-78.060716	0.000350
2.373	-232.978470	-154.955641	-78.059011	-154.955449	-78.058841	0.000361
2.329	-232.973625	-154.951336	-78.056401	-154.951138	-78.056227	0.000371
2.284	-232.969201	-154.946331	-78.053212	-154.946129	-78.053034	0.000380
2.243	-232.966078	-154.939989	-78.048799	-154.939783	-78.048617	0.000387
2.203	-232.964634	-154.932597	-78.043386	-154.932388	-78.043202	0.000393
2.158	-232.965486	-154.924748	-78.037556	-154.924536	-78.037370	0.000398
2.114	-232.969282	-154.915798	-78.030494	-154.915584	-78.030307	0.000401
2.070	-232.975754	-154.905924	-78.022683	-154.905708	-78.022495	0.000404
2.026	-232.984452	-154.895431	-78.014296	-154.895214	-78.014107	0.000405
1.982	-232.994716	-154.884495	-78.005563	-154.884278	-78.005375	0.000406
1.937	-233.005943	-154.873358	-77.996736	-154.873140	-77.996548	0.000407
1.893	-233.017623	-154.862223	-77.988046	-154.862004	-77.987858	0.000408
1.849	-233.029344	-154.851261	-77.979699	-154.851040	-77.979510	0.000409
1.805	-233.040765	-154.840600	-77.971853	-154.840379	-77.971663	0.000412
1.761	-233.051577	-154.830343	-77.964642	-154.830119	-77.964450	0.000416
1.717	-233.061476	-154.820579	-77.958182	-154.820353	-77.957987	0.000422
1.675	-233.070147	-154.811400	-77.952620	-154.811169	-77.952421	0.000429
1.633	-233.077259	-154.802937	-77.948166	-154.802702	-77.947962	0.000439
1.594	-233.082498	-154.795443	-77.945207	-154.795202	-77.944997	0.000452
1.561	-233.085677	-154.789334	-77.944274	-154.789086	-77.944057	0.000465
1.543	-233.088347	-154.777357	-77.942397	-154.777106	-77.942178	0.000470
1.531	-233.099236	-154.755862	-77.886776	-154.755608	-77.886552	0.000478

Energies in a.u.
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J. Mex. Chem. Soc. **2024**, *68*(1)
Special Issue

ISSN-e 2594-0317

SCS-MP2/aug-cc-pVTZ 1+2 IRC E2 (correlation) energies

ethene:	-0.345812	**butadiene:**	-0.662395			
r	**complex**	**butadiene- fo**	**ethene-fo**	**butadiene**	**ethene**	**CC**
2.874	-1.024274	-0.664764	-0.346616	-0.663946	-0.345866	0.001568
2.834	-1.025210	-0.664884	-0.346663	-0.664028	-0.345878	0.001641
2.794	-1.026218	-0.665025	-0.346716	-0.664129	-0.345895	0.001717
2.753	-1.027306	-0.665191	-0.346777	-0.664254	-0.345917	0.001797
2.713	-1.028484	-0.665387	-0.346850	-0.664407	-0.345950	0.001879
2.672	-1.029763	-0.665618	-0.346936	-0.664594	-0.345994	0.001966
2.630	-1.031160	-0.665893	-0.347045	-0.664823	-0.346059	0.002056
2.589	-1.032694	-0.666223	-0.347179	-0.665105	-0.346147	0.002150
2.546	-1.034398	-0.666621	-0.347356	-0.665454	-0.346275	0.002248
2.504	-1.036304	-0.667110	-0.347587	-0.665892	-0.346454	0.002351
2.460	-1.038467	-0.667722	-0.347906	-0.666450	-0.346719	0.002459
2.417	-1.040905	-0.668483	-0.348330	-0.667155	-0.347086	0.002573
2.373	-1.043700	-0.669472	-0.348925	-0.668083	-0.347621	0.002692
2.329	-1.046652	-0.670628	-0.349679	-0.669178	-0.348313	0.002817
2.284	-1.049749	-0.672046	-0.350614	-0.670528	-0.349181	0.002952
2.243	-1.052407	-0.673655	-0.351774	-0.672075	-0.350277	0.003077
2.203	-1.054418	-0.675483	-0.353152	-0.673820	-0.351581	0.003234
2.158	-1.055439	-0.677485	-0.354656	-0.675745	-0.353004	0.003392
2.114	-1.054965	-0.679595	-0.356375	-0.677776	-0.354641	0.003554
2.070	-1.053290	-0.681892	-0.358269	-0.679991	-0.356448	0.003723
2.026	-1.050781	-0.684284	-0.360275	-0.682296	-0.358364	0.003899
1.982	-1.047893	-0.686732	-0.362363	-0.684654	-0.360358	0.004084
1.937	-1.044943	-0.689194	-0.364475	-0.687020	-0.362373	0.004276
1.893	-1.042131	-0.691627	-0.366568	-0.689350	-0.364365	0.004479
1.849	-1.039559	-0.693999	-0.368595	-0.691614	-0.366288	0.004693
1.805	-1.037271	-0.696286	-0.370522	-0.693783	-0.368106	0.004920
1.761	-1.035276	-0.698466	-0.372317	-0.695837	-0.369785	0.005160
1.717	-1.033565	-0.700520	-0.373947	-0.697757	-0.371295	0.005415
1.675	-1.032122	-0.702426	-0.375371	-0.699520	-0.372595	0.005683
1.633	-1.030922	-0.704147	-0.376528	-0.701090	-0.373623	0.005962
1.594	-1.029936	-0.705607	-0.377302	-0.702397	-0.374268	0.006245
1.561	-1.029126	-0.706671	-0.377523	-0.703319	-0.374375	0.006500
1.543	-1.027650	-0.708378	-0.377818	-0.704982	-0.374616	0.006599
1.531	-1.025284	-0.726070	-0.385504	-0.722706	-0.382267	0.006601

Energies in a.u.
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J. Mex. Chem. Soc. **2024**, *68*(1)
Special Issue

ISSN-e 2594-0317

SCS-MP2/aug-cc-pVTZ 1+3 IRC RHF energies

ethene:	-78.064611	**Cp**	-192.859116			
r	**complex**	**Cp-fo**	**ethene-fo**	**Cp**	**ethene**	**CC**
2.981	-270.908363	-192.858543	-78.064658	-192.858381	-78.064544	0.000276
2.942	-270.906890	-192.858358	-78.064650	-192.858190	-78.064533	0.000285
2.903	-270.905276	-192.858126	-78.064637	-192.857953	-78.064517	0.000294
2.864	-270.903510	-192.857842	-78.064619	-192.857663	-78.064495	0.000304
2.824	-270.901578	-192.857494	-78.064593	-192.857308	-78.064465	0.000314
2.785	-270.899465	-192.857069	-78.064555	-192.856877	-78.064422	0.000324
2.744	-270.897159	-192.856556	-78.064502	-192.856358	-78.064365	0.000335
2.704	-270.894639	-192.855932	-78.064424	-192.855728	-78.064282	0.000346
2.663	-270.891895	-192.855179	-78.064313	-192.854968	-78.064166	0.000358
2.622	-270.888901	-192.854260	-78.064149	-192.854043	-78.063996	0.000370
2.580	-270.885652	-192.853145	-78.063910	-192.852921	-78.063752	0.000383
2.538	-270.882116	-192.851769	-78.063551	-192.851538	-78.063386	0.000396
2.495	-270.878311	-192.850078	-78.063019	-192.849841	-78.062848	0.000408
2.451	-270.874216	-192.847966	-78.062221	-192.847723	-78.062044	0.000421
2.407	-270.869932	-192.845362	-78.061060	-192.845112	-78.060877	0.000433
2.363	-270.865517	-192.842104	-78.059389	-192.841849	-78.059200	0.000444
2.318	-270.861323	-192.838256	-78.057050	-192.837996	-78.056856	0.000455
2.273	-270.857597	-192.833411	-78.054166	-192.833145	-78.053968	0.000463
2.230	-270.855054	-192.827920	-78.050322	-192.827651	-78.050120	0.000471
2.187	-270.854032	-192.821702	-78.045648	-192.821429	-78.045443	0.000477
2.142	-270.854957	-192.814401	-78.040476	-192.814125	-78.040269	0.000482
2.098	-270.858261	-192.806751	-78.034218	-192.806473	-78.034009	0.000486
2.053	-270.863732	-192.798271	-78.027336	-192.797990	-78.027127	0.000490
2.008	-270.871118	-192.789232	-78.019914	-192.788951	-78.019704	0.000492
1.963	-270.879858	-192.779744	-78.012110	-192.779461	-78.011899	0.000493
1.919	-270.889491	-192.769985	-78.004139	-192.769701	-78.003928	0.000495
1.874	-270.899529	-192.760110	-77.996193	-192.759825	-77.995982	0.000497
1.829	-270.909576	-192.750282	-77.988454	-192.749995	-77.988242	0.000499
1.784	-270.919261	-192.740645	-77.981068	-192.740355	-77.980854	0.000503
1.740	-270.928242	-192.731364	-77.974155	-192.731071	-77.973939	0.000509
1.696	-270.936169	-192.722640	-77.967824	-192.722342	-77.967604	0.000517
1.653	-270.942672	-192.714783	-77.962201	-192.714479	-77.961978	0.000527
1.611	-270.947361	-192.708410	-77.957504	-192.708099	-77.957275	0.000540
1.574	-270.949861	-192.705280	-77.954227	-192.704960	-77.953993	0.000554
1.561	-270.950244	-192.707982	-77.953188	-192.707654	-77.952952	0.000564

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Special Issue

ISSN-e 2594-0317

SCS-MP2/aug-cc-pVTZ 1+3 IRC E2 (correlation) energies

ethene:	-0.345812	**Cp**	-0.811445			
r	**complex**	**Cp-fo**	**ethene-fo**	**Cp**	**ethene**	**CC**
2.981	-1.172520	-0.812689	-0.346691	-0.811750	-0.345867	0.001763
2.942	-1.173351	-0.812786	-0.346731	-0.811805	-0.345874	0.001838
2.903	-1.174235	-0.812896	-0.346775	-0.811871	-0.345885	0.001915
2.864	-1.175176	-0.813022	-0.346824	-0.811951	-0.345898	0.001997
2.824	-1.176179	-0.813166	-0.346878	-0.812047	-0.345915	0.002082
2.785	-1.177253	-0.813331	-0.346940	-0.812162	-0.345938	0.002172
2.744	-1.178401	-0.813521	-0.347010	-0.812299	-0.345967	0.002265
2.704	-1.179637	-0.813741	-0.347093	-0.812465	-0.346006	0.002363
2.663	-1.180967	-0.813994	-0.347189	-0.812662	-0.346057	0.002464
2.622	-1.182414	-0.814294	-0.347307	-0.812903	-0.346128	0.002570
2.580	-1.183983	-0.814644	-0.347450	-0.813192	-0.346221	0.002681
2.538	-1.185715	-0.815070	-0.347635	-0.813555	-0.346354	0.002796
2.495	-1.187612	-0.815577	-0.347869	-0.813998	-0.346533	0.002916
2.451	-1.189735	-0.816209	-0.348186	-0.814564	-0.346791	0.003040
2.407	-1.192048	-0.816969	-0.348594	-0.815257	-0.347138	0.003169
2.363	-1.194602	-0.817925	-0.349144	-0.816143	-0.347624	0.003303
2.318	-1.197204	-0.819017	-0.349840	-0.817164	-0.348252	0.003441
2.273	-1.199819	-0.820384	-0.350693	-0.818459	-0.349034	0.003585
2.230	-1.201961	-0.821857	-0.351726	-0.819861	-0.349996	0.003726
2.187	-1.203443	-0.823478	-0.352934	-0.821411	-0.351130	0.003871
2.142	-1.204050	-0.825364	-0.354276	-0.823219	-0.352390	0.004031
2.098	-1.203451	-0.827260	-0.355814	-0.825034	-0.353843	0.004197
2.053	-1.201888	-0.829330	-0.357498	-0.827021	-0.355437	0.004370
2.008	-1.199560	-0.831469	-0.359281	-0.829072	-0.357128	0.004550
1.963	-1.196883	-0.833677	-0.361156	-0.831188	-0.358906	0.004739
1.919	-1.194094	-0.835900	-0.363066	-0.833313	-0.360716	0.004938
1.874	-1.191414	-0.838118	-0.364981	-0.835424	-0.362527	0.005149
1.829	-1.188948	-0.840294	-0.366861	-0.837486	-0.364297	0.005372
1.784	-1.186763	-0.842407	-0.368675	-0.839474	-0.365997	0.005611
1.740	-1.184882	-0.844425	-0.370397	-0.841358	-0.367599	0.005865
1.696	-1.183313	-0.846311	-0.372002	-0.843100	-0.369078	0.006136
1.653	-1.182051	-0.848009	-0.373459	-0.844641	-0.370402	0.006424
1.611	-1.181089	-0.849396	-0.374709	-0.845861	-0.371517	0.006726
1.574	-1.180453	-0.850122	-0.375616	-0.846421	-0.372294	0.007022
1.561	-1.180407	-0.849685	-0.375911	-0.845901	-0.372538	0.007156

Energies in a.u.
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