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SUPPLEMENTARY MATERIALS

*J. Am. Chem. Soc. JA973591A-3-a-346***Table S1.** Absolute energies (-au) of all species considered in the present study.

Species	BLYP/6-31G*	BLYP/6-311+G***a
1a	230.78812	230.86490
1b	309.38762	309.48337
4a	268.81861	-
4b	308.14968	-
4c	347.45546	347.55841
4d	386.74920	386.86360
4e	426.03494	426.16071
4f	465.32777	- ^b
TS1a	230.74785	230.81967
TS1b	309.33637	309.42665
TS4c	347.43466	347.53236
TS4d	386.71491	386.82383
TS4e	425.98940	426.10986
TS4f	465.26361	465.39623
2a (singlet)	230.76927	230.83682
2a (triplet)	230.77139	230.83629
2b (singlet)	270.00015	270.13828
2b (triplet)	270.06261	270.13846
2c (singlet)	309.34728	309.43577
2c (triplet)	309.35343	309.43996
5c	347.44429	347.54023
5d	386.72717	386.83448
5e	426.00118	426.12023
5f	465.26993	465.40093

^a BLYP/6-31G* geometries.^b Despite extensiv efforts, the energy at this level did not converge; comparisons in the text for this species are given at using the 6-311G** basis set instead.

Cartesian coordinates of all optimized structures.

Cartesian Coordinates (xmol format);
structures optimized at BLYP/6-31G*

10

1a

C 0.00000000 0.685238635 1.078273863
 C 0.00000000 0.685238635 1.078273863
 H 0.00000000 1.193889679 2.049528311
 H 0.00000000 1.193889679 2.049528311
 C 0.00000000 1.512764202 -0.073747647
 C 0.00000000 1.512764202 -0.073747647
 C 0.00000000 2.273868333 -1.030952908
 C 0.00000000 2.273868333 -1.030952908
 H 0.00000000 2.914087587 -1.890968164
 H 0.00000000 2.914087587 -1.890968164

16

1b

C 0.686193199 0.000000000 -1.746420415
 C -0.686193199 0.000000000 -1.746420415
 H 1.189371251 0.000000000 -2.721370733
 H -1.189371251 0.000000000 -2.721370733
 C 1.519235375 0.000000000 -0.598997501
 C -1.519235375 0.000000000 -0.598997501
 C 2.285320619 0.000000000 0.358305888
 C -2.285320619 0.000000000 0.358305888
 C 3.176357860 0.000000000 1.519578821
 C -3.176357860 0.000000000 1.519578821
 H 4.238975060 0.000000000 1.217065514
 H -4.238975060 0.000000000 1.217065514
 H 3.012204286 0.889845190 2.154752230
 H -3.012204286 0.889845190 2.154752230
 H 3.012204286 -0.889845190 2.154752230
 H -3.012204286 -0.889845190 2.154752230

11

4a

C -1.577548146 0.701160695 0.000000000
 C -1.577548320 0.701160303 0.000000000
 H -2.534647618 1.229266910 0.000000000
 H -2.534647924 1.229266279 0.000000000
 C -0.309277041 1.356907239 0.000000000
 C -0.309277379 1.356907162 0.000000000
 C 0.900686355 1.076057048 0.000000000
 C 0.900686087 1.076057272 0.000000000
 C 1.949123233 0.000000243 0.000000000
 H 2.604113402 -0.000000324 0.891324619
 H 2.604113402 -0.000000324 -0.891324619

14

4b

C -1.966102011 0.628628206 0.471618054
 C -1.983274597 -0.723121979 0.163911861
 H -2.883582033 1.157249189 0.745752907
 H -2.914750353 -1.295979711 0.187308186
 C -0.696465921 1.273506492 0.408493085
 C -0.729258052 -1.307620314 -0.179068221
 C 0.519678692 1.297090442 0.211517293

C 0.487030327 -1.273002624 -0.373511433
 C 1.871492860 0.835237848 -0.119547786
 C 1.851400033 -0.746162737 -0.479537909
 H 2.573733403 0.994324493 0.719036699
 H 2.261906398 -0.878624855 -1.497188884
 H 2.290695269 1.385110153 -0.981861240
 H 2.544989326 -1.269411282 0.203702672

17

4c

C 0.061391175 -2.318588488 0.692553978
 C 0.061391175 -2.318588488 -0.692553977
 H 0.119800711 -3.265423032 1.237280596
 H 0.119800711 -3.265423032 -1.237280595
 C -0.017656123 -1.071434825 1.373243170
 C -0.017656123 -1.071434825 -1.373243170
 C -0.095444657 0.153066471 1.461906694
 C -0.095444657 0.153066471 -1.461906694
 C -0.192560146 1.612006189 1.331639165
 C -0.192560146 1.612006189 -1.331639165
 C 0.450570139 2.135338292 -0.000000000
 H 1.522185169 1.875085165 -0.000000000
 H 0.376118645 3.238125076 -0.000000000
 H 0.301273979 2.127195458 2.177414736
 H 0.301273979 2.127195457 -2.177414736
 H -1.256318506 1.925311489 1.366693003
 H -1.256318506 1.925311489 -1.366693003

20

4d

C -2.574482664 0.685873236 0.075800630
 C -2.574711676 0.684943725 -0.076320463
 H -3.523383650 1.228237323 0.138168202
 H -3.523792951 -1.226957315 -0.138991633
 C -1.337956081 1.383156786 0.137244749
 C -1.338423858 1.382679391 -0.137371341
 C -0.152258501 1.701421932 0.133985935
 C -0.152839469 1.701367400 -0.134204866
 C 1.298864808 1.894041658 0.039949219
 C 1.298189546 1.894505178 -0.039732876
 H 1.528977305 2.734833446 -0.642797519
 H 1.527779878 -2.735404815 0.643057665
 H 1.719289430 2.183513105 1.023291219
 C 2.035923518 -0.613706037 0.485401454
 C 2.036319094 0.612968367 -0.484912926
 H 1.718830370 -2.184092438 -1.022947542
 H 1.581596980 -0.333590329 1.451017463
 H 1.582239051 0.333014706 -1.450692589
 H 3.078068320 -0.908297695 0.701872317
 H 3.078646965 0.907182531 -0.701014686

23

4e

C -2.845806825 0.678572471 0.116102139
 C -2.845464374 -0.679315414 -0.116122699
 H -3.797436710 1.212973482 0.206461562
 H -3.796826369 1.214177022 -0.206600992
 C -1.620248285 1.387870970 0.217896148

C-1.619580805-1.388053759-0.217733864
 C-0.456587932-1.777458833-0.243366789
 C-0.455870257-1.777461493-0.243632679
 C 0.960624055 2.131100477 0.112724957
 C 0.961344807-2.130984089-0.112588758
 H 1.043251466 3.135409262-0.345434645
 H 1.043876220-3.135136719 0.345934927
 H 1.437676815 2.223481946 1.108679732
 C 1.770054889-1.103433838 0.766753451
 C 1.769566585 1.103826763-0.766773161
 H 1.438648427-2.223694710-1.108392438
 H 1.087664276-0.657669213 1.509137269
 H 1.087221294 0.657811781-1.509042195
 C 2.545937809 0.000330570-0.000058054
 H 2.520206454-1.679421229 1.338644609
 H 2.519431270 1.680060522-1.338787920
 H 3.216272681-0.498153818-0.727397813
 H 3.216196178 0.499046762 0.727192281

26
 4f

C-2.877126354 0.687123914 0.001175286
 C-2.877126354-0.687123914-0.001175286
 C-1.707217833 1.489207508-0.003574144
 C-1.707217833-1.489207508 0.003574144
 C-0.690155587 2.176370083-0.014430144
 C-0.690155587-2.176370083 0.014430144
 C 0.605256333 2.868742748-0.045163106
 C 0.605256333-2.868742748 0.045163106
 C 1.785348863 1.951928078 0.416319388
 C 1.785348863-1.951928078-0.416319388
 H-3.846178198 1.200403453 0.002028324
 H-3.846178198-1.200403453-0.002028324
 H 0.803739298 3.229591407-1.074274116
 H 0.803739298-3.229591407 1.074274116
 H 0.572917614 3.774185139 0.590624281
 H 0.572917614-3.774185139 0.590624281
 H 1.620860693 1.697774721 1.478245401
 H 1.620860693-1.697774721-1.478245401
 H 2.713509210 2.549048577 0.378070904
 H 2.713509210-2.549048577-0.378070904
 C 1.922204814 0.646311687-0.427221961
 C 1.922204814-0.646311687 0.427221961
 H 2.834578897 0.685777416-1.050567749
 H 2.834578897-0.685777416 1.050567749
 H 1.070711069 0.580411526-1.126642480
 H 1.070711069-0.580411526 1.126642480

10

12a
 C 0.000000000 0.000000000 1.377727206
 C 0.000000000 1.201550519 0.743817440
 C 0.000000000 1.201550519-0.743817440
 C 0.000000000 0.000000000-1.377727206
 C 0.000000000-1.201550519-0.743817440
 C 0.000000000-1.201550519 0.743817440
 H 0.000000000 2.189621339 1.208083801
 H 0.000000000 2.189621339-1.208083801
 H 0.000000000-2.189621339-1.208083801
 H 0.000000000-2.189621339 1.208083801

10

32a
 C 0.000000000 0.000000000 1.332719622
 C 0.000000000 1.242817851 0.710738691
 C 0.000000000 1.242817851-0.710738691
 C 0.000000000 0.000000000-1.332719622
 C 0.000000000-1.242817851-0.710738691
 C 0.000000000-1.242817851 0.710738691
 H 0.000000000 2.181919830 1.274763997
 H 0.000000000 2.181919830-1.274763997
 H 0.000000000-2.181919830-1.274763997
 H 0.000000000-2.181919830 1.274763997

13

12b
 C 0.000002427-0.443087719 1.673639131
 C 0.000000118 1.040694608 1.648325101
 H 0.000003938-0.891744819 2.669056195
 H 0.000000099 1.527340873 2.625267585
 C 0.000002453-1.106735045 0.488048445
 C-0.000003227 1.640468231 0.426851172
 C 0.000000996-0.529701891-0.744660266
 C-0.000002812 0.969792620-0.749387196
 C 0.000000294-1.216424082-2.105185961
 H 0.000000280-2.308070773-1.983250235
 H-0.890095563-0.934512288-2.693584383
 H 0.890095569-0.934512432-2.693585162
 H-0.000005935 1.411459109-1.749686559

13

32b
 C 0.000003962-0.429292553 1.699969628
 C-0.000002160 0.990830055 1.700833158
 H 0.000004834-0.995664837 2.637747924
 H-0.000004613 1.559362210 2.636864911
 C 0.000003066-1.052387984 0.457958152
 C-0.000003491 1.601228679 0.451866887
 C 0.000000775-0.455110491-0.800473856
 C 0.000000665 0.972464176-0.784478942
 C-0.000001010-1.250319486-2.098172129
 H-0.000001606-2.332035458-1.894606973
 H-0.889036317-1.016880796-2.710253025
 H 0.889034151-1.016882443-2.710254256
 H-0.000007291 1.537626941-1.724515974

16

12c
 C 0.000000000-0.740344046 1.992705956
 C 0.000000000 0.740344046 1.992705956
 H 0.000000000-1.212009005 2.977180178
 H 0.000000000 1.212009005 2.977180178
 C 0.000000000-1.368278475 0.788004281
 C 0.000000000 1.368278475 0.788004281
 C 0.000000000-0.759785782-0.428181478
 C 0.000000000 0.759785782-0.428181478
 C 0.000000000-1.459623845-1.781800192
 C 0.000000000 1.459623845-1.781800192
 H 0.000000000-2.548150789-1.639381602
 H 0.000000000 2.548150789-1.639381602

H-0.887673646-1.190937381-2.381084990
 H-0.887673646 1.190937381-2.381084990
 H 0.887673646-1.190937381-2.381084990
 H 0.887673646 1.190937381-2.381084990

16

32c
 C 0.000000000-0.709715272 2.024619129
 C 0.000000000 0.709715272 2.024619129
 H 0.000000000-1.279913919 2.959792534
 H 0.000000000 1.279913919 2.959792534
 C 0.000000000-1.320630405 0.777336712
 C 0.000000000 1.320630405 0.777336712
 C 0.000000000-0.718603539-0.476983262
 C 0.000000000 0.718603539-0.476983262
 C 0.000000000-1.526692770-1.765696217
 C 0.000000000 1.526692770-1.765696217
 H 0.000000000-2.605265354-1.546184741
 H 0.000000000 2.605265354-1.546184741
 H-0.887815284-1.303208298-2.384632982
 H-0.887815284 1.303208298-2.384632982
 H 0.887815284-1.303208298-2.384632982
 H 0.887815284 1.303208298-2.384632982

11

4a
 C-1.577548146 0.701160695 0.000000000
 C-1.577548320-0.701160303 0.000000000
 H-2.534647618 1.229266910 0.000000000
 H-2.534647924-1.229266279 0.000000000
 C-0.309277041 1.356907239 0.000000000
 C-0.309277379-1.356907162 0.000000000
 C 0.900686355 1.076057048 0.000000000
 C 0.900686087-1.076057272 0.000000000
 C 1.949123233-0.000000243 0.000000000
 H 2.604113402-0.000000324 0.891324619
 H 2.604113402-0.000000324-0.891324619

14

4b
 C-1.966102011 0.628628206 0.471618054
 C-1.983274597-0.723121979 0.163911861
 H-2.883582033 1.157249189 0.745752907
 H-2.914750353-1.295979711 0.187308186
 C-0.696465921 1.273506492 0.408493085
 C-0.729258052-1.307620314-0.179068221
 C 0.519678692 1.297090442 0.211517293
 C 0.487030327-1.273002624-0.373511433
 C 1.871492860 0.835237848-0.119547786
 C 1.851400033-0.746162737-0.479537909
 H 2.573733403 0.994324493 0.719036699
 H 2.261906398-0.878624855-1.497188884
 H 2.290695269 1.385110153-0.981861240
 H 2.544989326-1.269411282 0.203702672

17

4c
 C 0.061391175-2.318588488 0.692553978
 C 0.061391175-2.318588488-0.692553977

H 0.119800711-3.265423032 1.237280596
 H 0.119800711-3.265423032-1.237280595
 C-0.017656123-1.071434825 1.373243170
 C-0.017656123-1.071434825-1.373243170
 C-0.095444657 0.153066471 1.461906694
 C-0.095444657 0.153066471-1.461906694
 C-0.192560146 1.612006189 1.331639165
 C-0.192560146 1.612006189-1.331639165
 C 0.450570139 2.135338292-0.000000000
 H 1.522185169 1.875085165-0.000000000
 H 0.376118645 3.238125076-0.000000000
 H 0.301273979 2.127195458 2.177414736
 H 0.301273979 2.127195457-2.177414736
 H-1.256318506 1.925311489 1.366693003
 H-1.256318506 1.925311489-1.366693003

20

4d
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 C-2.574711676-0.684943725-0.076320463
 H-3.523383650 1.228237323 0.138168202
 H-3.523792951-1.226957315-0.138991633
 C-1.337956081 1.383156786 0.137244749
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 C-0.152839469-1.701367400-0.134204866
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 C 1.298189546-1.894505178-0.039732876
 H 1.528977305 2.734833446-0.642797519
 H 1.5277779878-2.735404815 0.643057665
 H 1.719289430 2.183513105 1.023291219
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 C 2.036319094 0.612968367-0.484912926
 H 1.718830370-2.184092438-1.022947542
 H 1.581596980-0.333590329 1.451017463
 H 1.582239051 0.333014706-1.450692589
 H 3.078068320-0.908297695 0.701872317
 H 3.078646965 0.907182531-0.701014686

23

4e
 C-2.845806825 0.678572471 0.116102139
 C-2.845464374-0.679315414-0.116122699
 H-3.797436710 1.212973482 0.206461562
 H-3.796826369-1.214177022-0.206600992
 C-1.620248285 1.387870970 0.217896148
 C-1.619580805-1.388053759-0.217733864
 C-0.456587932 1.777458833 0.243366789
 C-0.455870257-1.777461493-0.243632679
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 C 0.961344807-2.130984089-0.112588758
 H 1.043251466 3.135409262-0.345434645
 H 1.043876220-3.135136719 0.345934927
 H 1.437676815 2.223481946 1.108679732
 C 1.770054889-1.103433838 0.766753451
 C 1.769566585 1.103826763-0.766773161
 H 1.438648427-2.223694710-1.108392438
 H 1.087664276-0.657669213 1.509137269
 H 1.087221294 0.657811781-1.509042195
 C 2.545937809 0.000330570-0.000058054
 H 2.520206454-1.679421229 1.338644609

H 2.519431270 1.680060522-1.338787920
H 3.216272681-0.498153818-0.727397813
H 3.216196178 0.499046762 0.727192281

26
4f

C-2.877126354 0.687123914 0.001175286
C-2.877126354-0.687123914-0.001175286
C-1.707217833 1.489207508-0.003574144
C-1.707217833-1.489207508 0.003574144
C-0.690155587 2.176370083-0.014430144
C-0.690155587-2.176370083 0.014430144
C 0.605256333 2.868742748-0.045163106
C 0.605256333-2.868742748 0.045163106
C 1.785348863 1.951928078 0.416319388
C 1.785348863-1.951928078-0.416319388
H-3.846178198 1.200403453 0.002028324
H-3.846178198-1.200403453-0.002028324
H 0.803739298 3.229591407-1.074274116
H 0.803739298-3.229591407 1.074274116
H 0.572917614 3.774185139 0.590624281
H 0.572917614-3.774185139-0.590624281
H 1.620860693 1.697774721 1.478245401
H 1.620860693-1.697774721-1.478245401
H 2.713509210 2.549048577-0.378070904
H 2.713509210-2.549048577-0.378070904
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C 1.922204814-0.646311687 0.427221961
H 2.834578897 0.685777416-1.050567749
H 2.834578897-0.685777416 1.050567749
H 1.070711069 0.580411526-1.126642480
H 1.070711069-0.580411526 1.126642480

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TS1a

C-1.229868620 0.706353609 0.000000000
C-1.229868620-0.706353609 0.000000000
H-2.193244677 1.221136649 0.000000000
H-2.193244677-1.221136649 0.000000000
C-0.002540827 1.387703801 0.000000000
C-0.002540827-1.387703801 0.000000000
C 1.220817147 1.038728158 0.000000000
C 1.220817147-1.038728158 0.000000000
H 2.262798479 1.320913857 0.000000000
H 2.262798479-1.320913857 0.000000000

16

TS1b

C-2.028188645 0.710569287-0.002317299
C-2.028188645-0.710569287 0.002317299
H-2.994407332 1.219908725-0.003952427
H-2.994407332-1.219908725 0.003952427
C-0.807242528 1.384164496-0.004546723
C-0.807242528-1.384164496 0.004546723
C 0.421249483 0.981623931-0.003259179
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H 2.388435364-1.180752814 0.892056180

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TS4c

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X-2.339706421-0.004333496 0.564407349
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C-2.338912964-0.710006714 0.564865112
C-1.145538330 1.370117188 0.331176758
C-1.142486572-1.376464844 0.332977295
X 0.034973145-0.002044678 0.106369019
C 0.036010742-0.934265137 0.1067979370
C 0.033935547 0.930175781 0.105758667
C 1.464782715-1.231323242-0.205047607
C 1.462036133 1.229949951-0.206665039
C 2.292648315 0.000473022 0.197814941
H-3.281112671 1.203994751 0.763916016
H-3.278427124-1.214462280 0.765502930
H 1.787384033-2.137771606 0.318405151
H 1.782623291 2.137771606 0.315597534
H 1.572448730-1.425018311-1.282852173
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H 3.281112671 0.001251221-0.272415161
H 2.434707642 0.001327515 1.284698486

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TS4d

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C 1.181448209 1.579369427-0.092862122
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C 2.349543935 0.678233351-0.364731282
C 2.349543935-0.678233351 0.364731282
H-3.618568141 1.221767959 0.015619114
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H 1.364904566 1.885827706 1.142002228
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H 2.292450504 0.513200331-1.456794554
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TS4e

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C-1.736374577-1.375733563-0.012280259
C-0.499341639 0.983436195 0.005813674
C-0.499341639-0.983436195-0.005813674
C 0.846289608 1.673632959-0.002271025
C 0.846289608-1.673632959 0.002271025

C 1.992019185 1.014390386 0.812221470
C 1.992019185-1.014390386-0.812221470
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H 0.657866980 2.684010790 0.395695945
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H 1.564640233 0.535886613 1.710447531
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H 2.663268077 1.810102639 1.181178181
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TS4f

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C-2.086926041-1.379234058 0.019205725
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C-0.852544979-0.982766051 0.038436793
C 0.499055446 1.613618315-0.250656617
C 0.499091343-1.613672139 0.250343875
C 1.648690941 1.360600056 0.789364313
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H 1.913299454 2.332152160 1.241106441
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C 2.930322132-0.762733574-0.148512073
H 3.794486914 0.976676075 0.804242624
H 3.794832540-0.977245775-0.803342874
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H 3.125679187-1.314408139 0.791494837

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23

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H-1.630069133 0.806926314-1.631171877
H-2.648290649-2.000520799 0.827005761
H-2.648290515 2.000521033-0.827005525
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26

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 H-0.521679110 1.756153101-2.111542810
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6d

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6f

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 C-1.954388218-1.383184581-0.055437922
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 C-0.709625974-0.711854334-0.023763872
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 H 2.763027610 0.541219644-1.443414533
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