

Electronic Supplementary Information

For

Theoretical study on the effective dehydrochlorination of 1,2-dichloroethane catalyzed
by tetraalkylphosphonium chlorides: electrostatically controlled reactivity

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Abbreviations used in the manuscript:

DFT: density functional theory

IL: ionic liquid

$C_{mmmm(n)}P^+Cl^-$: symmetrical and asymmetrical tetraalkylphosphonium chlorides, $m=1-4$, $n=1, 3, 14$

$C_{mmmm}P^+Cl^-$: symmetrical tetraalkylphosphonium chlorides, $m=1-4$

$C_{444,n}P^+Cl^-$: asymmetrical tetraalkylphosphonium chlorides, $n=1, 3, 14$

$C_{1111}P^+Cl^-$: tetramethylphosphonium chloride

$C_{2222}P^+Cl^-$: tetraethylphosphonium chloride

$C_{3333}P^+Cl^-$: tetrapropylphosphonium chloride

$C_{4444}P^+Cl^-$: tetrabutylphosphonium chloride

$C_{444,1}P^+Cl^-$: tributyltetramethylphosphonium chloride

$C_{444,3}P^+Cl^-$: tributyltetrapropyl phosphonium chloride

$C_{444,14}P^+Cl^-$: tributyltetradecylphosphonium chloride

$Bmin^+Cl^-$: 1-butyl-3-methyl imidazolium chloride

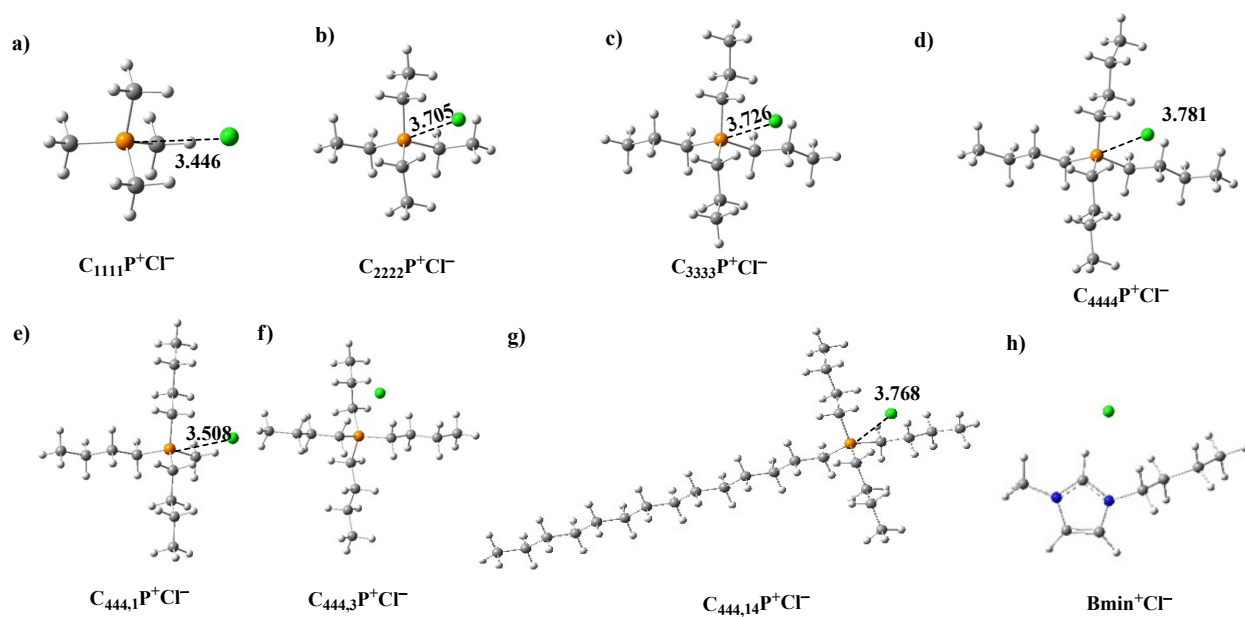


Fig. S1 Optimized structures of symmetrical tetraalkylphosphonium chlorides (a-d), asymmetrical tetraalkylphosphonium chlorides (e-g), and $Bmin^+Cl^-$ ionic pair (h).

Cartesian coordinates of all structures optimized in this work:

$C_{1111}P^+Cl^-$:

P	0.84433200	0.00056700	-0.00077900
C	2.67367400	-0.00181300	0.00045800
H	3.05005700	0.76971400	0.67732900
H	3.04644500	-0.97470200	0.33151900
H	3.05010200	0.19696100	-1.00647000
C	0.27567500	-1.29126800	-1.13570600
H	0.63490300	-2.26711700	-0.79742000
H	-0.82427800	-1.24380500	-1.10376200
H	0.64877400	-1.09202900	-2.14404100
C	0.27780800	1.63047700	-0.55028700
H	-0.82215500	1.57899800	-0.53353800
H	0.64430700	2.40056700	0.13396600
H	0.64548400	1.83159400	-1.56029900
C	0.27659000	-0.33757800	1.68604100
H	0.64659400	0.43544400	2.36523600
H	-0.82337000	-0.32347600	1.63271600
H	0.64071400	-1.31630900	2.00996100
Cl	-2.60147300	-0.00019200	0.00020300

$C_{2222}P^+Cl^-$:

P	-0.59288100	-0.00001500	0.15392600
C	0.01289500	-0.00157300	1.88919500
C	1.53192300	-0.00410200	2.10942000
H	-0.45275300	-0.87757100	2.35736900
H	-0.44991100	0.87557700	2.35801300
H	1.72809900	-0.00443100	3.18658000
H	2.01144300	-0.87135500	1.65414000
H	2.01445100	0.86130300	1.65383000
C	-0.06289400	-1.48539100	-0.76200800
C	-0.28666900	-2.81610900	-0.03352300
H	1.00880300	-1.29250500	-0.97324700
H	-0.59194500	-1.46161600	-1.72209800
H	0.05010100	-3.63363600	-0.67643600
H	0.29892700	-2.87058200	0.88841500
H	-1.33775900	-3.00320600	0.21336600
C	-2.43047700	-0.00009300	0.33146700
C	-3.21346100	0.00123200	-0.98830800
H	-2.69145800	0.87706200	0.93439100
H	-2.69154700	-0.87840300	0.93266400
H	-4.28756100	0.00101600	-0.78274200
H	-2.99324800	0.88681400	-1.59089400

H	-2.99322600	-0.88313300	-1.59267200
C	-0.06295400	1.48683500	-0.75965700
C	-0.28588400	2.81636400	-0.02874100
H	-0.59261300	1.46487400	-1.71945600
H	1.00860100	1.29409900	-0.97178700
H	0.05075900	3.63487900	-0.67046300
H	-1.33675400	3.00340800	0.21913800
H	0.30034900	2.86906800	0.89289600
Cl	2.91915200	0.00150500	-1.02629200

$C_{3333}P^+Cl^-$:

P	0.40955100	-0.00112900	0.20322900
C	2.14213700	-0.00432600	0.83798200
C	3.24526100	-0.00101000	-0.23357500
H	2.24351100	-0.88511800	1.48378600
H	2.24451300	0.87156900	1.49026700
C	4.64663200	-0.00613200	0.38700000
H	3.13243800	-0.87572200	-0.88446200
H	3.13511000	0.88020100	-0.87606000
H	5.41630000	-0.00356800	-0.39028300
H	4.80553000	0.87537600	1.01734900
H	4.80282600	-0.89414000	1.00884300
C	-0.61382000	-0.00039000	1.72754500
C	-2.14446500	-0.00532900	1.56957300
H	-0.28784400	0.87928400	2.29810900
H	-0.28258700	-0.87473700	2.30325600
C	-2.83446900	0.00301100	2.93684000
H	-2.46502800	0.84846500	0.96735500
H	-2.46012700	-0.87098200	0.98177500
H	-3.92092400	-0.00132200	2.81238700
H	-2.56430400	-0.87636900	3.53371900
H	-2.56990900	0.89334500	3.51979900
C	0.12776600	1.48167900	-0.81956400
C	0.14715500	2.82462000	-0.07245300
H	-0.85311100	1.28562200	-1.29898200
H	0.88676600	1.46034000	-1.61192800
C	-0.09104300	3.99087600	-1.03874700
H	-0.63913300	2.82826200	0.69132600
H	1.09995900	2.97291500	0.45434500
H	-0.10252200	4.94551400	-0.50387400
H	0.69537500	4.04164200	-1.79965900
H	-1.04890400	3.87490800	-1.55400200
C	0.12308200	-1.48159800	-0.82170600
C	0.14014000	-2.82568000	-0.07656300

H	0.88128800	-1.46094600	-1.61484900
H	-0.85761300	-1.28218200	-1.29997200
C	-0.10466300	-3.98987500	-1.04367300
H	1.09404000	-2.97769300	0.44716000
H	-0.64377200	-2.82783300	0.68966800
H	-0.11742700	-4.94519200	-0.51004200
H	-1.06374300	-3.87030000	-1.55583100
H	0.67921300	-4.04206600	-1.80710600
Cl	-2.71090900	0.00779900	-1.83273500

C₄₄₄₄P⁺Cl⁻:

P	-0.36077100	-0.02401700	-0.21794400
C	-0.15454400	-1.48740000	0.84701300
C	0.06581300	-2.82468500	0.12430000
H	-1.03905600	-1.52878900	1.49530300
H	0.70852600	-1.21414700	1.48993800
C	0.23262600	-3.97716400	1.12630900
H	-0.76705000	-3.05378700	-0.55613600
H	0.96953200	-2.76388800	-0.49470500
C	0.49196900	-5.32308300	0.44447900
H	1.05829300	-3.73432500	1.80508500
H	-0.66887200	-4.04572900	1.74961100
H	0.60421900	-6.12366900	1.18189500
H	-0.33220300	-5.59962400	-0.22352200
H	1.40921300	-5.29386600	-0.15414600
C	0.91380800	0.04017400	-1.53737200
C	2.38344600	0.12339200	-1.09180500
H	0.64992700	0.90099500	-2.16559700
H	0.74565900	-0.85094100	-2.15598600
C	3.33035700	0.17534900	-2.29811100
H	2.53587800	0.99493800	-0.44833000
H	2.63175300	-0.72324000	-0.44494600
C	4.80117300	0.26225800	-1.87964000
H	3.17716600	-0.71428200	-2.92568000
H	3.07547200	1.03884700	-2.92924600
H	5.45987600	0.30138300	-2.75314700
H	4.98627500	1.15612200	-1.27539800
H	5.09089200	-0.60321000	-1.27528000
C	-1.95693100	-0.10848300	-1.13634700
C	-3.22512800	-0.16384800	-0.26922300
H	-1.90239100	-0.98941000	-1.78774500
H	-1.98743900	0.76529300	-1.79886200
C	-4.50424400	-0.22520000	-1.11709600

H	-3.18863500	-1.03927400	0.39092900
H	-3.26856300	0.71586400	0.38474400
C	-5.77756000	-0.27924400	-0.26844500
H	-4.53934300	0.64929200	-1.78025700
H	-4.46033200	-1.10459700	-1.77319100
H	-6.67033100	-0.32375000	-0.89929100
H	-5.78481100	-1.16124000	0.38123400
H	-5.86615400	0.60525900	0.37172900
C	-0.31270500	1.45308600	0.84622300
C	-0.25361300	2.80721500	0.12412400
H	0.57902600	1.27860100	1.48413800
H	-1.19120000	1.39300200	1.50135500
C	-0.21109200	3.96926800	1.12783100
H	0.64445900	2.85003100	-0.50463700
H	-1.11456900	2.93921400	-0.54745500
C	-0.11826100	5.33873400	0.45015600
H	-1.10755900	3.93051400	1.76100200
H	0.64423500	3.82310000	1.79766100
H	-0.09376300	6.14364400	1.19103100
H	0.79021600	5.42040300	-0.15682600
H	-0.97582700	5.51955100	-0.20851000
Cl	2.37519700	0.12469200	2.38753000

$C_{444,1}P^+Cl^-$:

P	-0.03150300	-0.19213800	0.45888300
C	-1.53042200	-0.40313200	-0.56205600
C	-2.86498600	-0.16730100	0.16200800
H	-1.44794300	-1.45060800	-0.89897600
H	-1.42520800	0.25983100	-1.42991600
C	-4.05794700	-0.35569900	-0.78700300
H	-2.95786300	-0.88098600	0.98897100
H	-2.90829400	0.83968700	0.60111200
C	-5.40666300	-0.16194300	-0.08889200
H	-3.96967000	0.34972700	-1.62425700
H	-4.00494200	-1.36068900	-1.22200800
H	-6.23678100	-0.30733300	-0.78682400
H	-5.53357500	-0.87760600	0.73069900
H	-5.49882800	0.84611700	0.33193900
C	0.13556400	1.56693200	0.97721400
C	0.29349800	2.58468700	-0.16416500
H	0.99442900	1.61723800	1.65753200
H	-0.74922000	1.80342100	1.58081600
C	0.41667600	4.02565400	0.35201400
H	1.18021000	2.33921300	-0.76194800

H	-0.56549700	2.51871700	-0.84380700
C	0.57871300	5.04892700	-0.77540700
H	-0.47111000	4.27169200	0.94943400
H	1.27306800	4.09158800	1.03605700
H	0.66505400	6.06434200	-0.37740100
H	1.47695300	4.84677200	-1.36906000
H	-0.27978600	5.03034700	-1.45575900
C	1.41229200	-0.69599600	-0.53679600
C	2.77639100	-0.58574600	0.16092100
H	1.38943100	-0.10138800	-1.45853200
H	1.17079300	-1.74232900	-0.79382700
C	3.91529900	-1.05178400	-0.75826200
H	2.97293300	0.44636600	0.48424200
H	2.77635400	-1.20611200	1.06551500
C	5.28999700	-0.97077100	-0.08943500
H	3.71411100	-2.08227600	-1.07388700
H	3.91302500	-0.44309800	-1.67253300
H	6.07892000	-1.30843800	-0.76834300
H	5.52864600	0.05562800	0.21275900
H	5.33248900	-1.59976300	0.80651100
C	-0.14204800	-1.19003000	1.97142200
H	-0.25870500	-2.23097400	1.63020600
H	0.76986100	-1.07352500	2.56239900
H	-1.00128500	-0.87200900	2.56699100
Cl	-0.37371900	-3.57789800	-0.39533700

$C_{444,3}P^+Cl^-$:

P	0.00067000	0.08548700	0.29874800
C	-1.46559600	-0.13682100	-0.76203800
C	-2.82766200	-0.02242100	-0.06056600
H	-1.30156800	-1.12885600	-1.22755500
H	-1.37743700	0.60157700	-1.56898700
C	-3.98331800	-0.26626700	-1.04304300
H	-2.89261800	-0.75687100	0.75209300
H	-2.95118100	0.96709200	0.40235300
C	-5.35880400	-0.17188100	-0.37770200
H	-3.91782700	0.46195600	-1.86220900
H	-3.85475900	-1.25392700	-1.50100200
H	-6.15970600	-0.35254500	-1.10100100
H	-5.46387200	-0.91161200	0.42382600
H	-5.52450200	0.81900900	0.06103100
C	0.00567500	1.77965400	1.02583100
C	0.08559200	2.93452000	0.01419500
H	0.85036900	1.82447300	1.72419500

H	-0.90377900	1.86681300	1.63253600
C	0.05984500	4.30988500	0.69680200
H	1.00296700	2.84525500	-0.58043700
H	-0.74993100	2.86898200	-0.69400900
C	0.14265200	5.46859000	-0.30081000
H	-0.85848200	4.40058900	1.29190100
H	0.89324900	4.37502200	1.40875500
H	0.12050000	6.43421500	0.21302200
H	1.06780100	5.42413300	-0.88582600
H	-0.69631600	5.44702000	-1.00492900
C	1.48877500	-0.15449700	-0.72608000
C	2.82893600	-0.18972000	0.02357700
H	1.47682100	0.64852000	-1.47403000
H	1.28859400	-1.10611200	-1.26182300
C	4.00513800	-0.34173600	-0.95313200
H	2.97625200	0.71625300	0.62981600
H	2.83871200	-1.03890900	0.71777500
C	5.35934100	-0.42514000	-0.24412200
H	3.84315300	-1.24068600	-1.55909100
H	4.00493600	0.50546400	-1.65189600
H	6.17566100	-0.53173400	-0.96497200
H	5.55678500	0.47423500	0.35097400
H	5.40025300	-1.28655300	0.43166800
C	-0.02481600	-1.03635500	1.75472500
H	0.96852600	-0.94254000	2.21191800
H	-0.73073200	-0.59212200	2.46853600
C	-0.36384900	-2.51698200	1.50085400
H	0.21817500	-2.90744400	0.65927300
H	-1.40630900	-2.59660600	1.17540800
C	-0.15051600	-3.35394400	2.76540500
H	-0.41609600	-4.39807900	2.57773100
H	0.89742600	-3.33264300	3.08650500
H	-0.76242100	-2.99793700	3.60334600
Cl	0.09229100	-2.93229700	-1.93232300

C_{444,14}P⁺Cl⁻:

P	-3.93806600	0.03611200	0.15858900
C	-4.10372700	-1.40857500	-0.94086800
C	-4.04478500	-2.78377100	-0.25806300
H	-3.31372500	-1.31304700	-1.69657300
H	-5.06044800	-1.22722100	-1.46829300
C	-4.22890700	-3.92079300	-1.27454600
H	-3.08879000	-2.92173100	0.26711600
H	-4.83155400	-2.85709700	0.50316300

C	-4.19137700	-5.30797200	-0.62798900
H	-5.18136700	-3.77639800	-1.79774900
H	-3.44501000	-3.84822800	-2.03995400
H	-4.32314300	-6.09532100	-1.37631600
H	-3.23619100	-5.48790100	-0.12098900
H	-4.98829400	-5.42152500	0.11541700
C	-5.17408900	0.00961900	1.52011300
C	-6.62175200	-0.35520200	1.14250400
H	-5.13332400	1.00981700	1.96973000
H	-4.78010100	-0.68023500	2.27741000
C	-7.58957700	-0.08676100	2.30219100
H	-6.93249900	0.18235100	0.23831800
H	-6.66449400	-1.41602200	0.86815000
C	-9.02739200	-0.48871200	1.95990700
H	-7.25877200	-0.62333400	3.20350100
H	-7.55964700	0.98214200	2.55602800
H	-9.70993500	-0.26153100	2.78515700
H	-9.37924300	0.04078400	1.06924900
H	-9.09852700	-1.56204500	1.75276000
C	-2.30603700	0.00145400	1.01429700
C	-1.07251800	0.03146200	0.09708100
H	-2.29416100	-0.90000300	1.63883500
H	-2.29132600	0.85542600	1.70268100
C	0.24195200	0.00610200	0.89054200
H	-1.09765800	-0.82584700	-0.58701900
H	-1.09678500	0.93006000	-0.53138700
C	1.48653400	0.02096700	-0.00543700
H	0.27045800	0.86844400	1.57105900
H	0.26263400	-0.88753600	1.52975700
H	1.45634500	-0.84445000	-0.68221300
H	1.45955900	0.91083900	-0.64984200
C	-4.07559900	1.54186600	-0.85889400
C	-4.12866000	2.87427600	-0.09683300
H	-4.99305100	1.37092700	-1.46060900
H	-3.22539700	1.51918500	-1.55265800
C	-4.19629300	4.06361600	-1.06689600
H	-5.01756700	2.89519600	0.54555100
H	-3.25811900	2.99505300	0.56459900
C	-4.29204500	5.41227900	-0.34899400
H	-3.30899000	4.05144800	-1.71391400
H	-5.06046500	3.92837900	-1.72761500
H	-4.33722600	6.23764400	-1.06602100
H	-5.19120500	5.46647300	0.27467700
H	-3.42568900	5.58365400	0.30065500

C	2.80301100	0.00411300	0.78128900
H	2.82626400	-0.88236200	1.43090300
H	2.83465200	0.87302600	1.45383200
C	4.04849700	0.00950400	-0.11350800
H	4.01718500	-0.86138800	-0.78352100
H	4.02254400	0.89365900	-0.76614400
C	5.36619800	-0.00224600	0.67106100
H	5.39029700	-0.88450600	1.32653500
H	5.39855100	0.87068300	1.33854600
C	6.61158700	-0.00215900	-0.22385100
H	6.57956700	-0.87626900	-0.88977700
H	6.58593700	0.87872200	-0.88106200
C	7.93005900	-0.01080600	0.55946300
H	7.95486600	-0.89068600	1.21815800
H	7.96273200	0.86441800	1.22398700
C	9.17510100	-0.01349700	-0.33591800
H	9.14260800	-0.88939100	-0.99953100
H	9.14931400	0.86557000	-0.99560700
C	10.49416200	-0.02027500	0.44641500
H	10.51959500	-0.89891100	1.10681000
H	10.52696900	0.85619000	1.10936600
C	11.73889400	-0.02423600	-0.44910800
H	11.70721400	-0.90102600	-1.11183300
H	11.71400600	0.85400400	-1.11018900
C	13.05864800	-0.03010700	0.33215300
H	13.08360700	-0.90772900	0.99245300
H	13.09068800	0.84640400	0.99362000
C	14.29596800	-0.03448900	-0.57043900
H	15.22059600	-0.03857500	0.01584300
H	14.30990500	-0.91770200	-1.21920200
H	14.31696900	0.84941500	-1.21806000
Cl	-6.78450100	0.23308800	-2.30298000

Bmin⁺Cl⁻:

C	1.37156100	0.22941500	-0.10097800
C	2.49970000	-1.68129700	0.07305700
C	1.25422500	-1.96735900	-0.39917600
N	0.57335500	-0.76752500	-0.50346500
H	1.01515100	1.29868900	-0.07052300
H	3.33931300	-2.32274300	0.28767800
H	0.80426400	-2.90849500	-0.67155300
N	2.54991600	-0.30689500	0.25357700
C	3.69116200	0.46418900	0.74355900
H	3.97816300	0.11404000	1.73756000

H	4.53633600	0.36002000	0.05928100
H	3.39687400	1.51192200	0.79998500
C	-0.83159200	-0.56760000	-0.92381200
C	-1.81136000	-0.73952300	0.23801800
H	-1.02639400	-1.27701100	-1.73408000
H	-0.89057600	0.45917900	-1.29814600
C	-3.25512300	-0.48521800	-0.21251900
H	-1.71829500	-1.74588200	0.67018600
H	-1.54235800	-0.01239300	1.01224300
C	-4.26458900	-0.65196800	0.92662700
H	-3.31789500	0.53274300	-0.61452500
H	-3.51276500	-1.16752000	-1.03487900
H	-5.28479800	-0.45842800	0.58119600
H	-4.23923500	-1.66763100	1.33850700
H	-4.05235700	0.04556400	1.74361500
Cl	-0.31013100	2.77382600	-0.18388100

Na⁺Cl⁻:

Cl	0.00000000	0.00000000	0.93346400
Na	0.00000000	0.00000000	-1.44262600

Following are the cartesian coordinates of the optimized intermediates, transition states and products.

1:

C	0.6549	0.90342	-0.37921
H	1.20114	1.81991	-0.14365
H	0.49947	0.84017	-1.4565
C	-0.65488	0.90343	0.37921
H	-0.49946	0.84018	1.4565
H	-1.20114	1.8199	0.14362
Cl	-1.73996	-0.47533	-0.0808
Cl	1.73995	-0.47533	0.0808

TS₁₋₂:

C	0.12222	1.3271	-0.33025
H	0.77487	2.0915	0.07978
H	0.12301	1.17542	-1.40499
C	-0.6625	0.55812	0.53488
H	0.38906	-0.11149	0.60912
H	-0.87143	0.92167	1.53976
Cl	-1.93973	-0.47595	-0.11493
Cl	2.10598	-0.42925	-0.00575

2:

C	-0.5592	1.57752	-0.28802
H	-0.08218	2.44515	0.15786
H	-0.59844	1.51336	-1.37025
C	-1.10726	0.65854	0.50431
H	1.36473	0.21846	0.02796
H	-1.10189	0.70728	1.58796
Cl	-1.9346	-0.75957	-0.10004
Cl	2.54733	-0.31694	-0.00004

3:

C	-0.59326600	0.86529900	-0.06867300
H	-0.04851700	1.70185200	0.37443400
H	-0.52620600	0.91235600	-1.15557900
C	-2.02579200	0.88996500	0.41562800
H	-2.09451000	0.71865900	1.49021000
H	-2.45803500	1.86419800	0.17462000
Cl	-3.06635500	-0.35449400	-0.39094000
Cl	0.28746800	-0.64707000	0.44183700
Cl	3.85156700	0.08728800	-0.22609500
H	2.60604500	-0.18595000	0.01295500

TS₃₋₄:

C	0.41787600	-1.43778500	0.78125300
H	-0.15081800	-1.70252500	1.66750300
H	0.53439600	-2.19179000	0.01100700
C	1.11070700	-0.22046400	0.75836400
H	0.25918000	0.64362300	0.53924800
H	1.45124100	0.14482600	1.73294800
C1	2.34826300	0.00784400	-0.50256000
C1	-1.93713500	-1.10754900	-0.36432800
C1	-0.97569400	1.85101700	0.10417500
H	-1.66787300	0.28304900	-0.22229500

4:

C	1.28017100	-1.48616700	0.29287100
H	0.66756500	-1.95465400	1.05748700
H	1.09037800	-1.73990900	-0.74489300
C	2.26615000	-0.66888900	0.66169900
H	0.10059200	0.49294900	0.32713300
H	2.49471800	-0.42039000	1.69286900
C1	3.34602900	0.10550900	-0.47288400
C1	-3.89697100	-0.58077400	-0.21481000
C1	-0.78982300	1.44000300	0.21757300
H	-2.83817100	0.15180900	-0.06796100

5:

C1	-3.25741400	-0.48576500	-0.07949200
C	0.09161000	0.34180100	0.64761000
H	0.44971500	0.38150300	1.67672000
H	-1.00532500	0.33635600	0.60484800
C	0.57030000	-0.89451300	-0.07242400
H	0.15962300	-1.77366500	0.42747500
H	0.25717900	-0.89585900	-1.11572000
C1	2.38384600	-1.08830700	-0.06926500
C1	0.64811800	1.88395000	-0.14797500

TS₅₋₆:

C1	-0.68884600	2.24799100	0.01388800
C	0.59540800	-1.23310800	0.82435200
H	0.86284300	-2.06535800	0.19055800
H	1.17367300	-1.10481700	1.73010300
C	-0.63869500	-0.60487000	0.73578400
H	-1.14372500	-0.33621400	1.66122100
H	-0.50553400	0.75457000	0.33379700
C1	-1.81393200	-1.26217700	-0.45905400

C1	2.49527600	-0.17524400	-0.33580400
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6:

C1	1.57898100	1.72898800	0.00032600
C	-1.01937700	-1.24956600	0.00211300
H	-1.52897000	-2.20744700	0.00244900
H	0.06783400	-1.22439900	0.00197300
C	-1.66265900	-0.09071000	0.00085100
H	-1.16584100	0.87274100	0.00098000
H	2.20703100	0.28541500	-0.00056100
C1	-3.42643400	0.03850500	-0.00092300
C1	2.81875700	-1.16070900	-0.00073300

7:

P	1.45834500	0.21974700	0.48042700
C	1.05157200	0.63322800	-1.24900400
C	2.21809800	1.14920300	-2.10742200
H	0.24313600	1.37327500	-1.19913100
H	0.60295900	-0.28511500	-1.66303500
C	1.75042700	1.51266300	-3.52493300
H	2.68496600	2.02979900	-1.64581100
H	3.00027100	0.38303700	-2.17738100
C	2.89102800	2.00998100	-4.41658600
H	1.27696800	0.63354100	-3.97898700
H	0.97037500	2.28232100	-3.45928500
H	2.52704200	2.26030100	-5.41769900
H	3.36068500	2.90778500	-3.99917900
H	3.67053800	1.24796800	-4.52720900
C	2.82031700	-1.00589700	0.55937600
C	2.44707200	-2.44620800	0.16127000
H	3.21852100	-0.97266300	1.58081200
H	3.61369300	-0.61575900	-0.08997100
C	3.69312300	-3.33287800	0.03349500
H	1.77605800	-2.86808900	0.91888600
H	1.87092600	-2.45689600	-0.77089900
C	3.34637300	-4.78791700	-0.29367100
H	4.34675800	-2.92576900	-0.74982100
H	4.27268900	-3.29212800	0.96603000
H	4.25065300	-5.39591400	-0.39631700
H	2.73115400	-5.23471600	0.49507700
H	2.78352200	-4.85784700	-1.23029600
C	2.06279500	1.71178900	1.36614800
C	1.09831100	2.91035500	1.37152900
H	3.01779300	1.98820000	0.90277700

H	2. 29641000	1. 40008500	2. 39132400
C	1. 67373900	4. 10788600	2. 14190500
H	0. 87791300	3. 21722400	0. 34183700
H	0. 14045900	2. 61960200	1. 82041400
C	0. 72912300	5. 31292400	2. 14870100
H	1. 89135400	3. 80255300	3. 17365900
H	2. 63547300	4. 39374200	1. 69650900
H	1. 16364900	6. 14941700	2. 70407200
H	0. 52147100	5. 66057200	1. 13078900
H	-0. 22924400	5. 06389500	2. 61737600
C	-0. 05203300	-0. 43119100	1. 26994500
C	0. 09585500	-0. 86033900	2. 73908400
H	-0. 37007000	-1. 26023200	0. 61816700
H	-0. 81584900	0. 34854100	1. 16229500
C	-1. 22315000	-1. 41462600	3. 29825500
H	0. 87436100	-1. 62809400	2. 83267400
H	0. 42008000	-0. 01257800	3. 35694000
C	-1. 10988600	-1. 85714300	4. 75943100
H	-2. 00325900	-0. 64799400	3. 20423600
H	-1. 54569300	-2. 26021900	2. 67785300
H	-2. 06344700	-2. 24863100	5. 12646100
H	-0. 35859100	-2. 64567000	4. 87886000
H	-0. 82147500	-1. 02191500	5. 40735400
C1	-0. 76521900	-2. 33738200	-1. 72889600
C	-3. 25278300	0. 07215200	-1. 78695800
H	-3. 81824600	0. 41538900	-2. 65321900
H	-2. 29480200	-0. 37117300	-2. 07754700
C	-3. 99512500	-0. 97273300	-0. 99303100
H	-4. 07676500	-1. 87376600	-1. 60306800
H	-3. 47485900	-1. 22311100	-0. 07041500
C1	-5. 69021600	-0. 48042000	-0. 54372200
C1	-2. 86879300	1. 56823300	-0. 80777700

TS₇₋₈:

P	-1. 24631500	0. 10121200	0. 71194300
C	-1. 45959600	0. 10990800	-1. 09866900
C	-2. 91510400	0. 14473400	-1. 59312800
H	-0. 91666400	-0. 77181200	-1. 46601900
H	-0. 88171300	0. 96503000	-1. 46849200
C	-2. 98354100	0. 15670500	-3. 12759800
H	-3. 46660300	-0. 72738100	-1. 21863600
H	-3. 43600600	1. 03024500	-1. 20532700
C	-4. 41963700	0. 18315400	-3. 65778200
H	-2. 43269800	1. 02820900	-3. 50341200

H	-2.45936400	-0.72589800	-3.51461800
H	-4.43543100	0.19194400	-4.75194300
H	-4.98334900	-0.69537200	-3.32424000
H	-4.95614400	1.07325600	-3.31028000
C	-1.97320100	1.61888900	1.44661200
C	-1.38738200	2.94319500	0.92522900
H	-1.84117900	1.53860700	2.53222300
H	-3.05338300	1.57562200	1.26259800
C	-2.02434700	4.15968700	1.61223700
H	-0.30248600	2.96273400	1.08185200
H	-1.53905400	3.01733000	-0.15815100
C	-1.46142100	5.48776500	1.09846600
H	-3.11113700	4.13433300	1.45790900
H	-1.86673100	4.08625300	2.69635300
H	-1.93163200	6.33639700	1.60446600
H	-0.38141200	5.55349600	1.26941000
H	-1.63475300	5.60243400	0.02289900
C	-2.15315100	-1.31057300	1.45443600
C	-1.68780600	-2.70389900	0.99508400
H	-3.21460000	-1.16049100	1.22195800
H	-2.05917500	-1.20939000	2.54256700
C	-2.49841000	-3.82182900	1.66612400
H	-1.77335800	-2.78897700	-0.09413600
H	-0.62324000	-2.83669400	1.21769200
C	-2.05242400	-5.21877700	1.22533700
H	-2.40605800	-3.73207900	2.75674400
H	-3.56368600	-3.68535000	1.43710700
H	-2.64425300	-5.99537200	1.71951000
H	-2.16672500	-5.34809900	0.14369300
H	-0.99921700	-5.39388200	1.46991200
C	0.53126100	-0.00701800	1.10561500
C	0.87309200	-0.08646600	2.60260800
H	1.00136500	0.85918800	0.62588500
H	0.90248800	-0.87837300	0.54872200
C	2.38882600	-0.20052900	2.82674100
H	0.49933700	0.79987100	3.13240800
H	0.37831700	-0.95259000	3.06117700
C	2.76350800	-0.27797600	4.30903900
H	2.76182400	-1.08761800	2.30036500
H	2.88697100	0.65814600	2.36000000
H	3.84734200	-0.35831300	4.43725600
H	2.42978500	0.61386100	4.85149500
H	2.30631100	-1.14966300	4.79078300
C1	1.64948600	1.89170200	-1.85607400

C	3. 50371300	-1. 39258800	-2. 34487300
H	3. 75868600	-2. 17116500	-1. 64194700
H	3. 20739000	-1. 70308800	-3. 33849000
C	3. 83244500	-0. 06527600	-2. 13404300
H	4. 16692200	0. 52344200	-2. 98654600
H	2. 66886300	0. 73677600	-1. 98620800
Cl	4. 77763200	0. 33630700	-0. 66153500
Cl	1. 20218900	-2. 21320800	-1. 66617400

8:

P	2. 09286600	0. 10313500	0. 39098000
C	1. 42092800	1. 08903400	-0. 99333900
C	2. 24723300	2. 32823000	-1. 37779200
H	0. 39731000	1. 36041600	-0. 70504100
H	1. 32531100	0. 39951800	-1. 84170800
C	1. 62319600	3. 07274200	-2. 56754400
H	2. 31549700	3. 01222200	-0. 51906300
H	3. 27643500	2. 03490700	-1. 63400200
C	2. 41723200	4. 32027200	-2. 96507200
H	1. 55415900	2. 38919200	-3. 42450900
H	0. 59231700	3. 35459700	-2. 31493000
H	1. 95134300	4. 82994100	-3. 81477600
H	2. 47255500	5. 03579400	-2. 13652200
H	3. 44367600	4. 06356700	-3. 25204600
C	3. 73346400	-0. 58784300	-0. 04387700
C	3. 75119500	-1. 52684500	-1. 26222300
H	4. 09597300	-1. 10731400	0. 85263300
H	4. 39985300	0. 26976600	-0. 20277200
C	5. 16277200	-2. 06483900	-1. 53876800
H	3. 06763100	-2. 37203800	-1. 09432700
H	3. 38409600	-0. 99403500	-2. 15178500
C	5. 20792800	-3. 00798300	-2. 74445100
H	5. 84558300	-1. 22019500	-1. 70345300
H	5. 53028600	-2. 58909800	-0. 64598400
H	6. 22356600	-3. 37830600	-2. 91810700
H	4. 55691600	-3. 87640800	-2. 59202300
H	4. 87649800	-2. 50045900	-3. 65757200
C	2. 33970500	1. 15351200	1. 87046700
C	1. 06961000	1. 82650900	2. 41931900
H	3. 09029200	1. 90465200	1. 59280400
H	2. 80186000	0. 51166700	2. 63145600
C	1. 37952300	2. 69752600	3. 64554300
H	0. 60592100	2. 44745200	1. 63897600
H	0. 32834400	1. 06158800	2. 69261100

C	0.13121400	3.38011500	4.21209200
H	1.84597400	2.07587300	4.42219300
H	2.12390100	3.45721800	3.37028400
H	0.37751200	3.99196000	5.08611800
H	-0.33533300	4.03398000	3.46651100
H	-0.61772000	2.64174300	4.52030700
C	0.90588800	-1.23881300	0.75049800
C	1.25881900	-2.11980900	1.96107700
H	0.83187400	-1.83783800	-0.16588100
H	-0.06972400	-0.75299000	0.87678800
C	0.21364200	-3.22453200	2.17499000
H	2.24897700	-2.57884300	1.82101900
H	1.32033000	-1.50114100	2.86848800
C	0.52866000	-4.10912400	3.38460500
H	-0.77538500	-2.76399800	2.30035200
H	0.15243900	-3.84358100	1.26976700
H	-0.23212900	-4.88579700	3.51417500
H	1.49827300	-4.60776900	3.27062600
H	0.56426700	-3.52001800	4.30836300
C1	-1.58189400	-1.20204200	-2.47327400
C	-5.85501200	-0.45403800	-0.92117300
H	-5.96854900	-1.23121200	-1.67152300
H	-4.85304700	-0.09565000	-0.69516700
C	-6.88728400	0.06911000	-0.27427000
H	-6.82532800	0.84855600	0.48460800
H	-1.89808200	-0.31070500	-1.38337500
C1	-8.55521700	-0.44023500	-0.56190400
C1	-2.26341500	0.76441800	-0.06533300