

Mononuclear palladium(II) and platinum(II) complexes of P- and C-donor ligands; synthesis, crystal structures, cytotoxicity, and mechanistic studies on a highly stereoselective Mizoroki–Heck reaction

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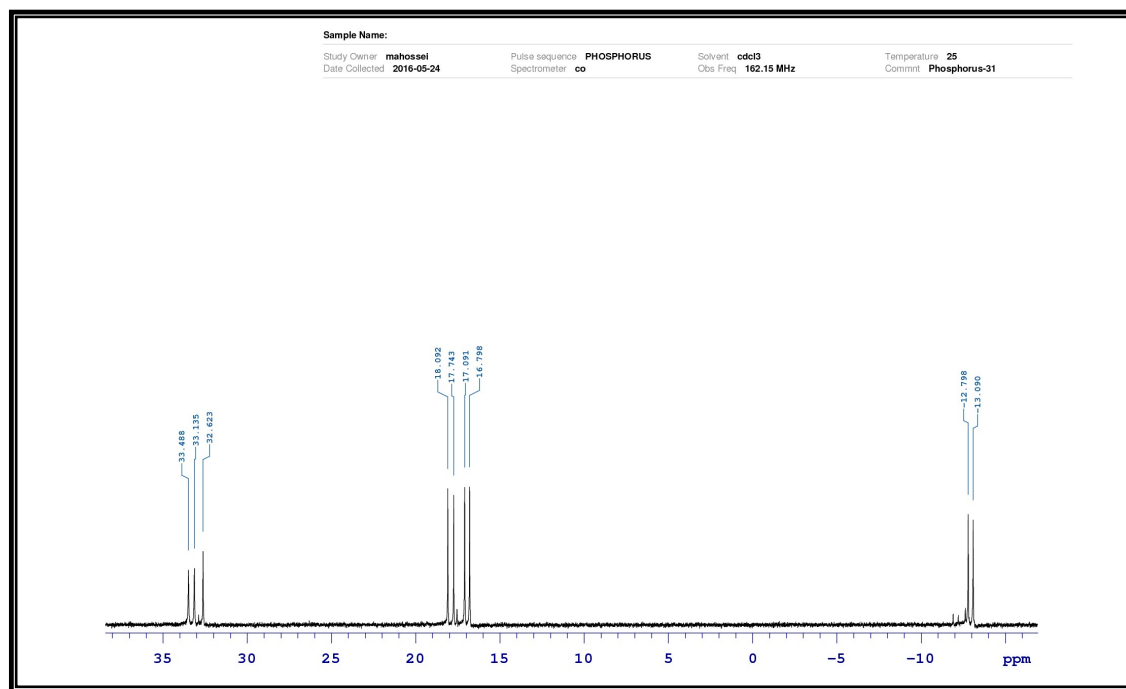
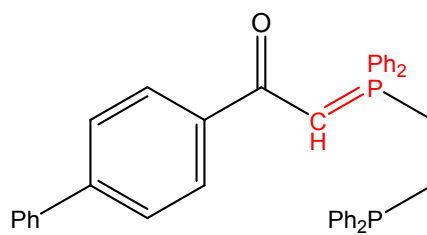


Figure S1. ^{31}P NMR of $\text{Ph}_2\text{P}(\text{CH}_2)_2\text{PPh}_2=\text{C}(\text{H})\text{C}(\text{O})\text{C}_6\text{H}_4\text{-}p\text{-Ph}$ (**Y1**).



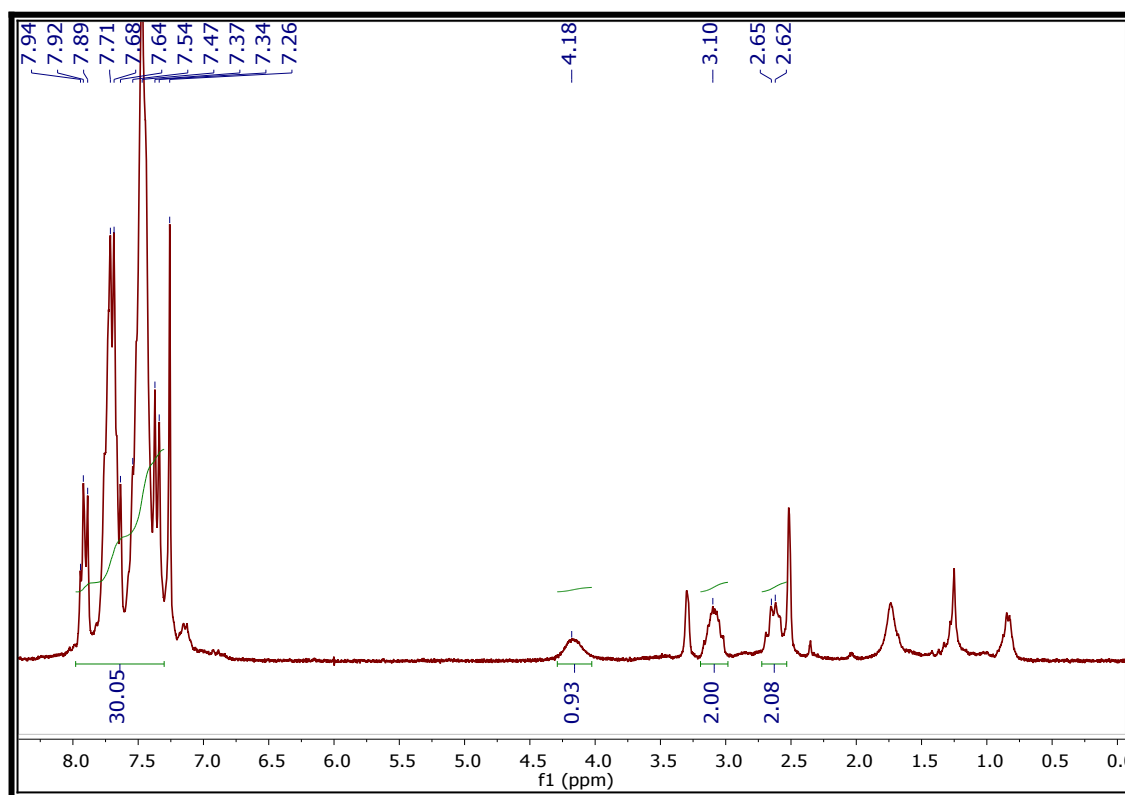
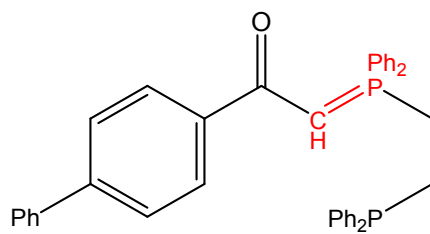


Figure S2. ^1H NMR of $\text{Ph}_2\text{P}(\text{CH}_2)_2\text{PPh}_2=\text{C}(\text{H})\text{C}(\text{O})\text{C}_6\text{H}_4\text{-}p\text{-Ph}$ (Y^1).



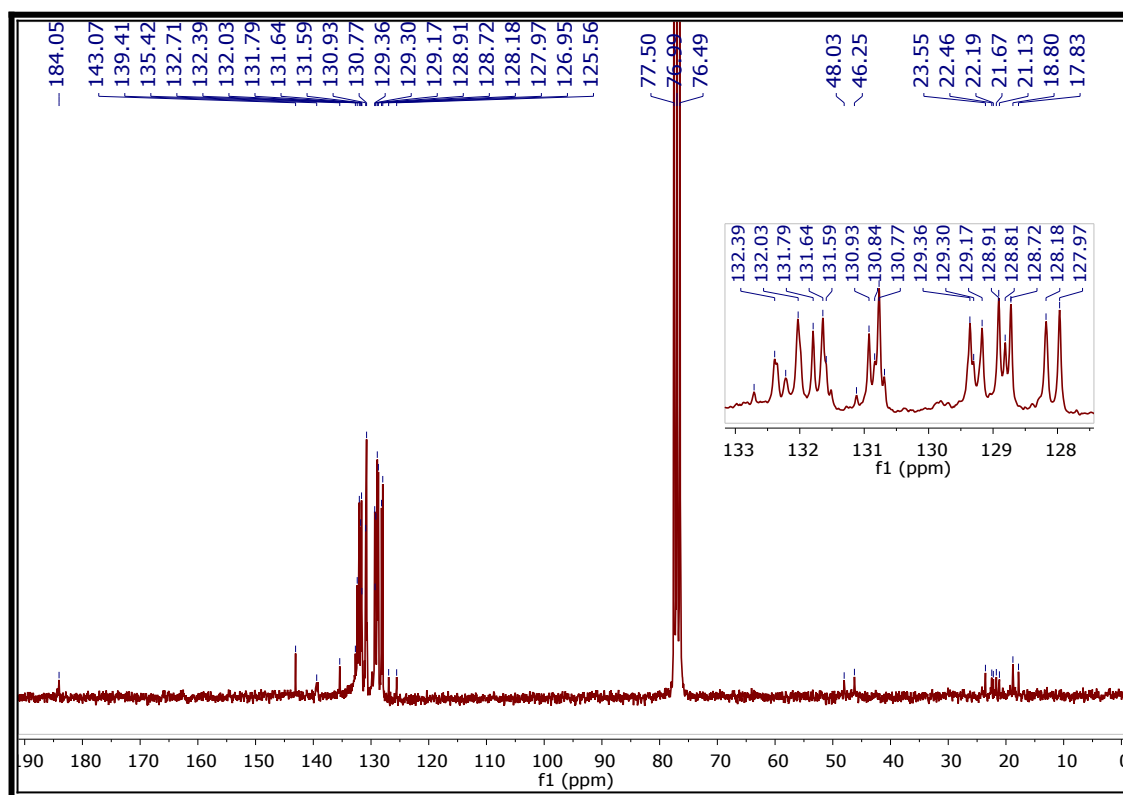
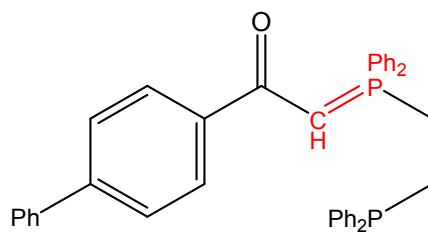


Figure S3. ^{13}C NMR of $\text{Ph}_2\text{P}(\text{CH}_2)_2\text{PPh}_2=\text{C}(\text{H})\text{C}(\text{O})\text{C}_6\text{H}_4\text{-}p\text{-Ph}$ (**Y1**).



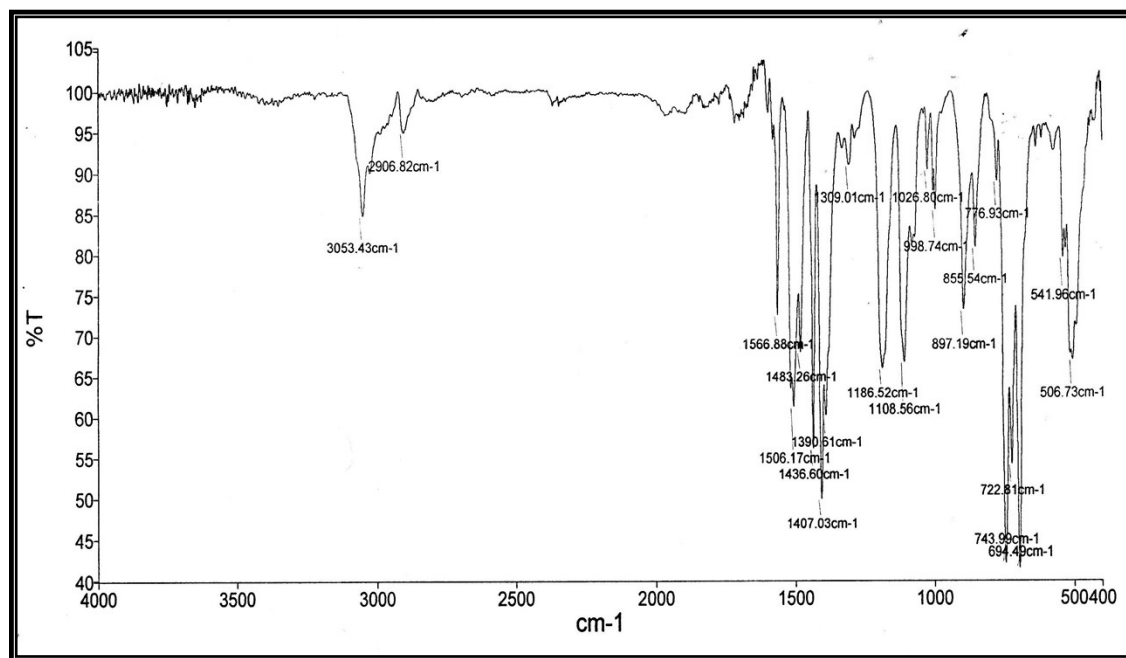
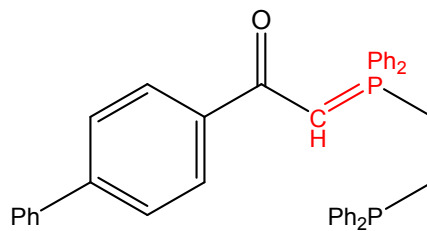


Figure S4. IR spectrum of $\text{Ph}_2\text{P}(\text{CH}_2)_2\text{PPh}_2=\text{C}(\text{H})\text{C}(\text{O})\text{C}_6\text{H}_4\text{-}p\text{-Ph}$ (Y^1).



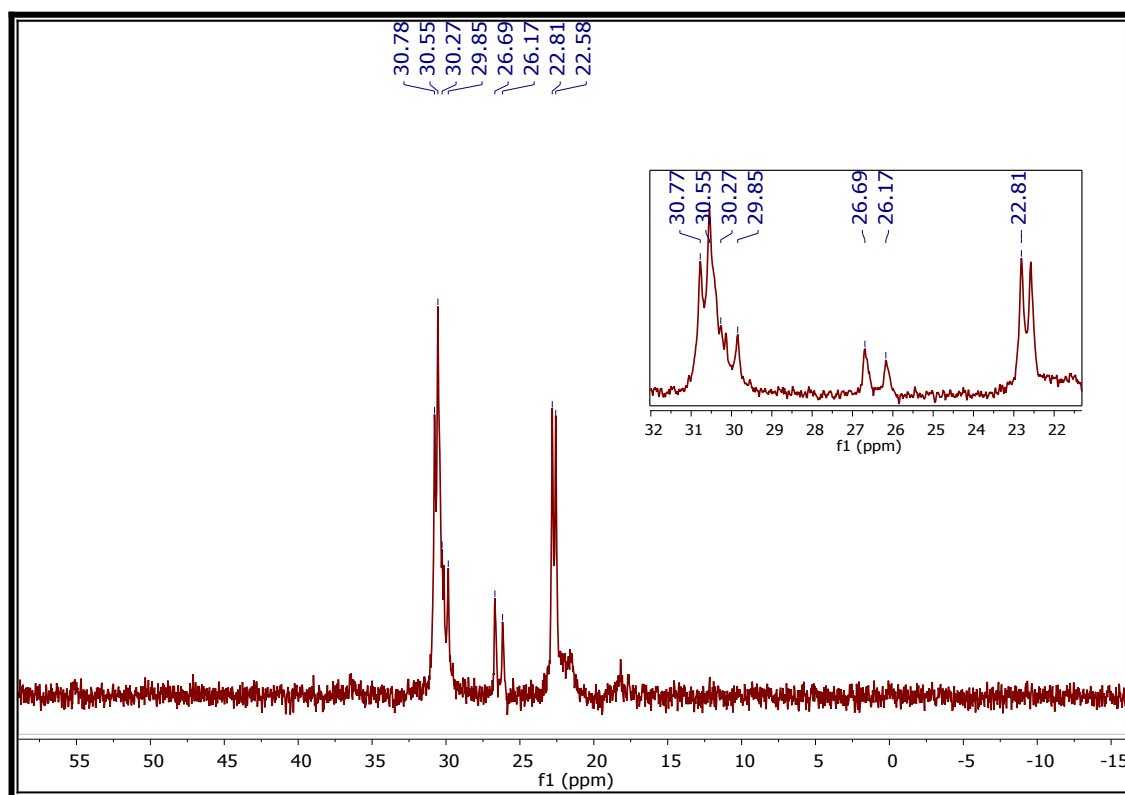
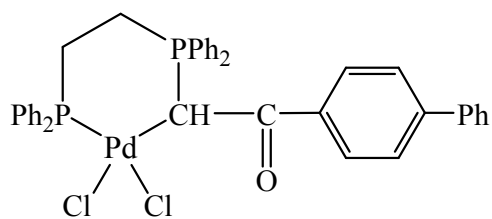


Figure S5. ^{31}P NMR of $[\text{PdCl}_2(\text{Ph}_2\text{P}(\text{CH}_2)_2\text{PPh}_2\text{C}(\text{H})\text{C}(\text{O})\text{C}_6\text{H}_4\text{-}p\text{-Ph})]$ (1).



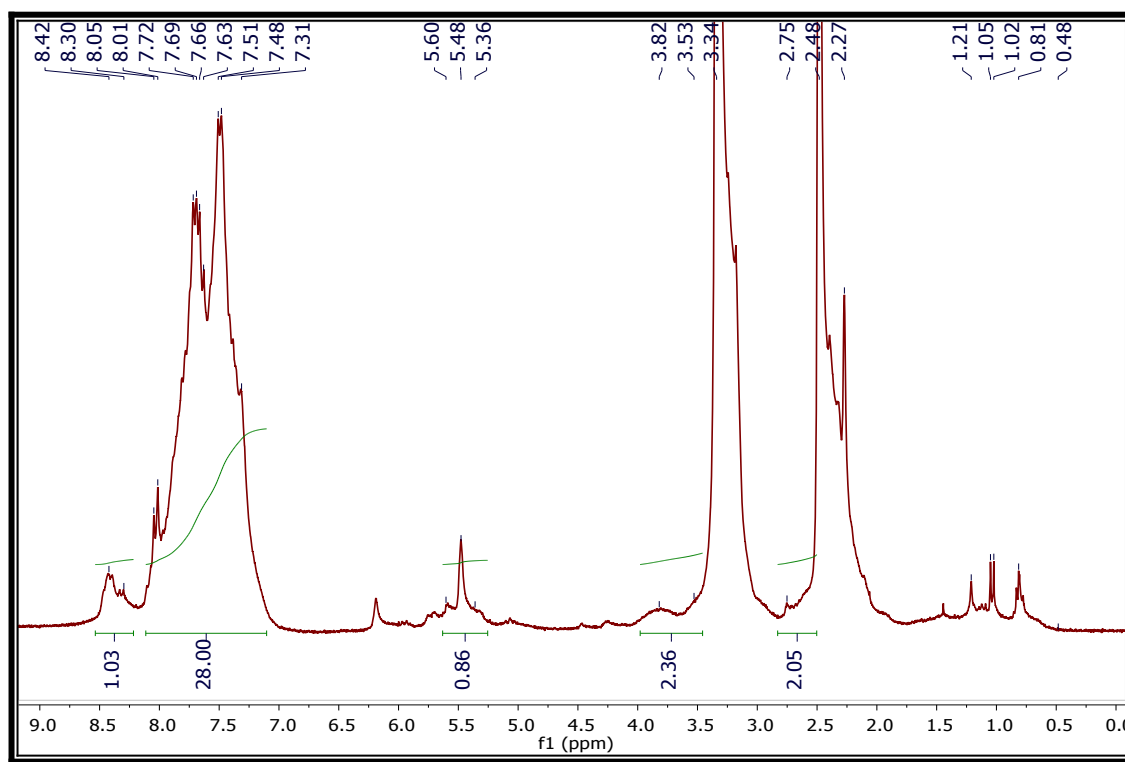
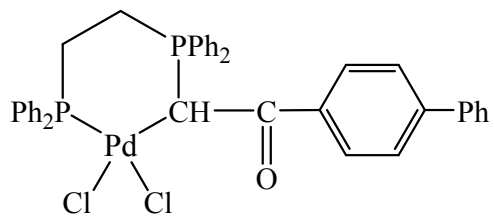


Figure S6. ¹H NMR of [PdCl₂(Ph₂P(CH₂)₂PPh₂C(H)C(O)C₆H₄-*p*-Ph)] (1).



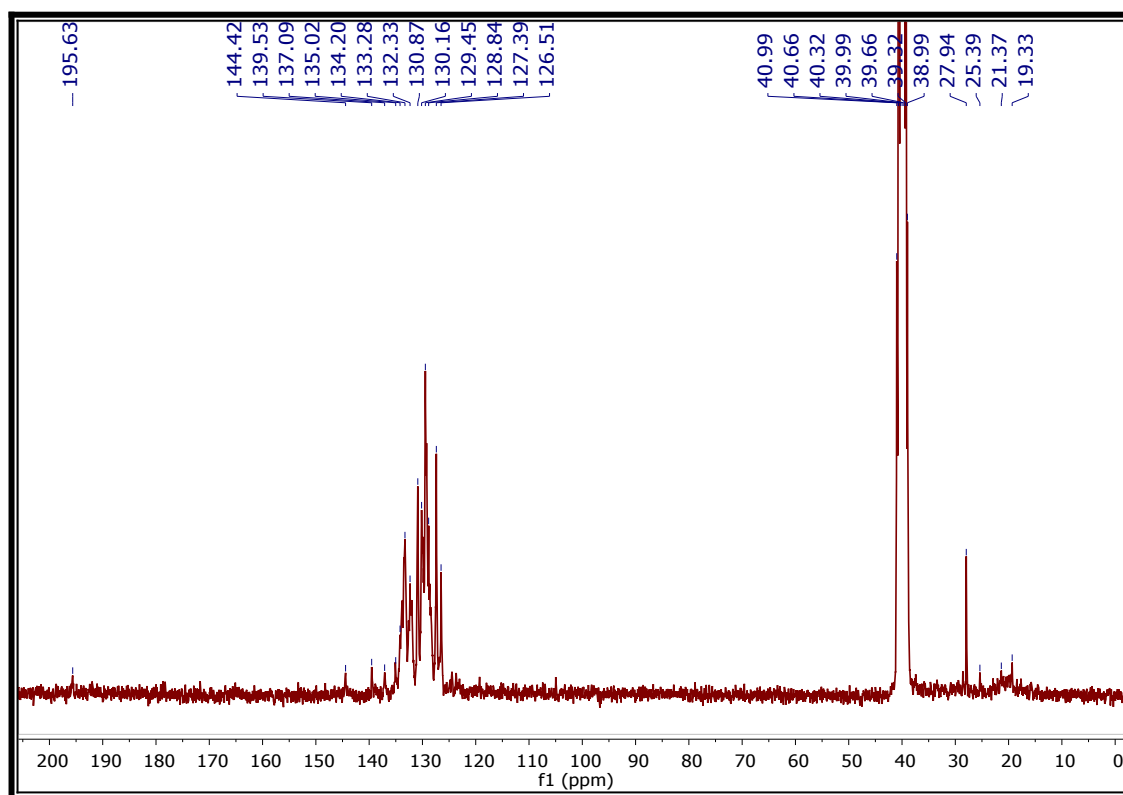
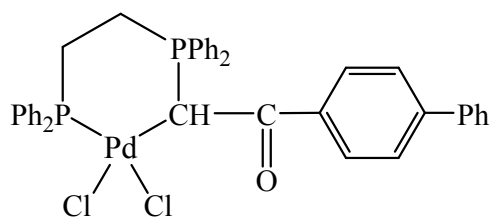


Figure S7. ^{13}C NMR of $[\text{PdCl}_2(\text{Ph}_2\text{P}(\text{CH}_2)_2\text{PPh}_2\text{C}(\text{H})\text{C}(\text{O})\text{C}_6\text{H}_4\text{-}p\text{-Ph})]$ (**1**).



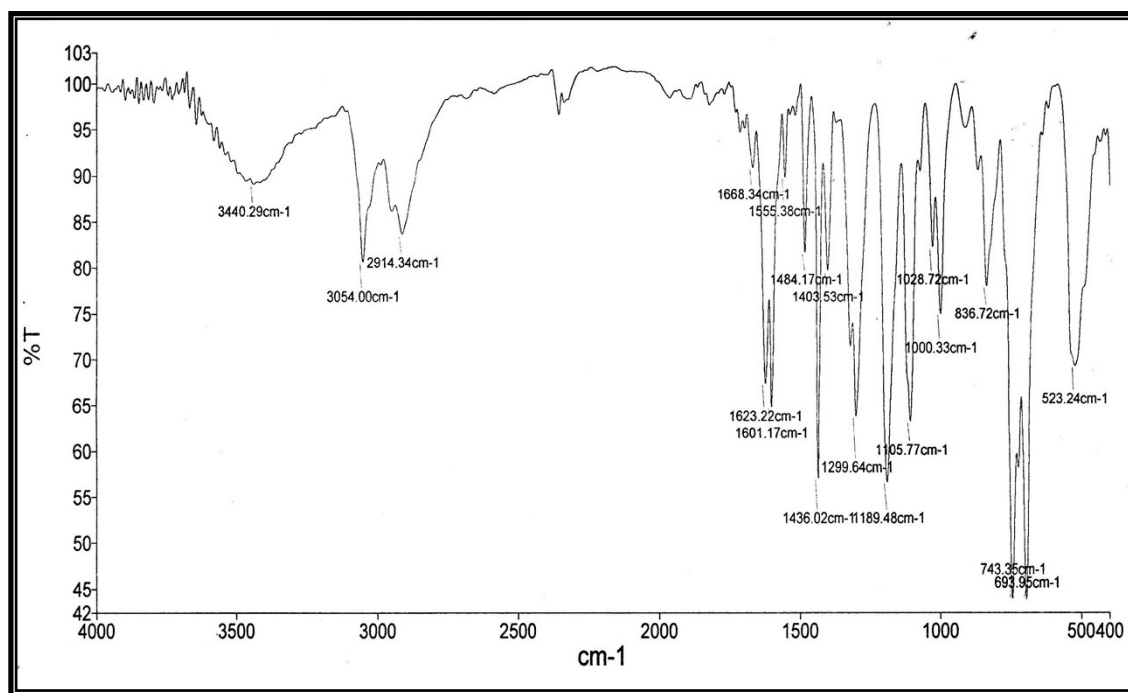
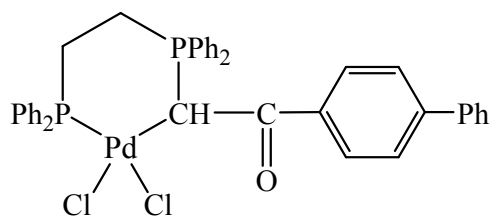


Figure S8. IR spectrum of $[\text{PdCl}_2(\text{Ph}_2\text{P}(\text{CH}_2)_2\text{PPh}_2\text{C}(\text{H})\text{C}(\text{O})\text{C}_6\text{H}_4\text{-}p\text{-Ph})]$ (**1**).



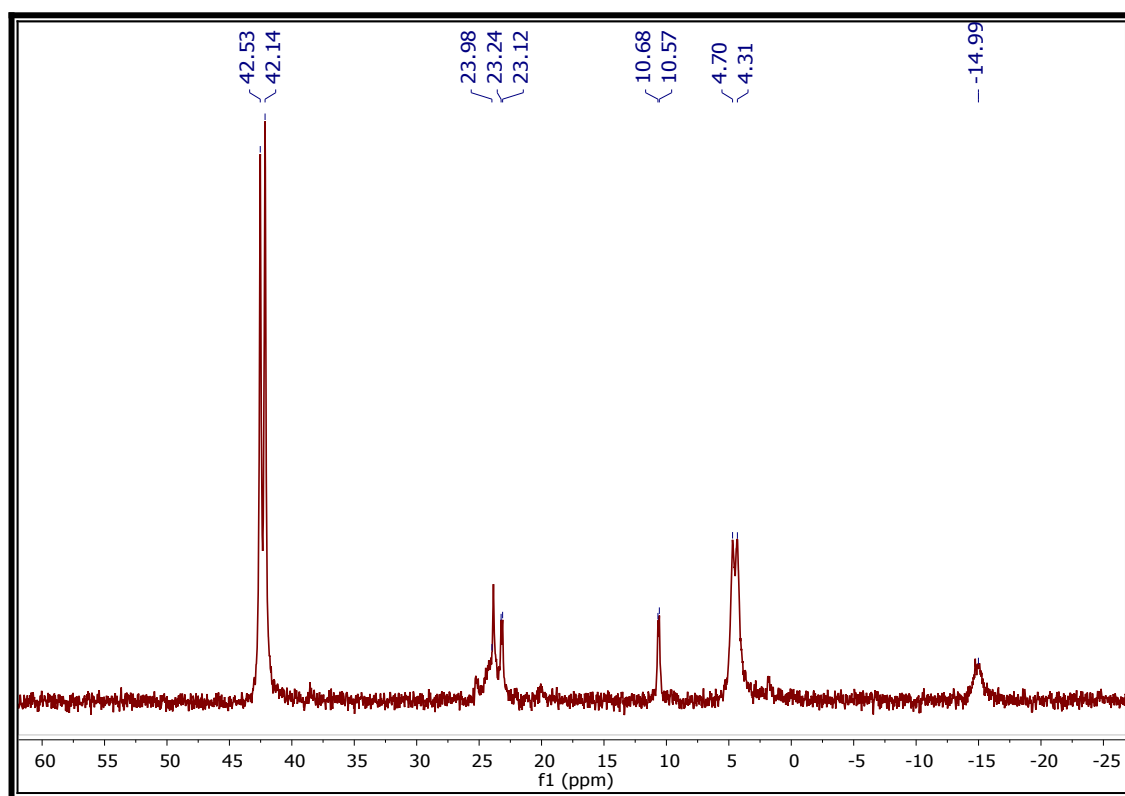
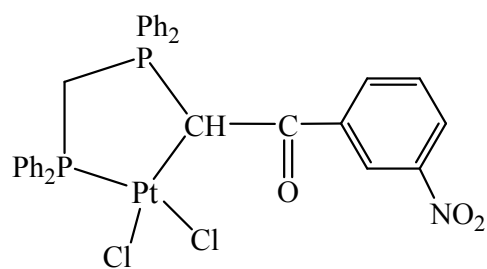


Figure S9. ^{31}P NMR of $[\text{PtCl}_2(\text{Ph}_2\text{PCH}_2\text{PPh}_2\text{C}(\text{H})\text{C}(\text{O})\text{C}_6\text{H}_4\text{-}m\text{-NO}_2)]$ (**2**).



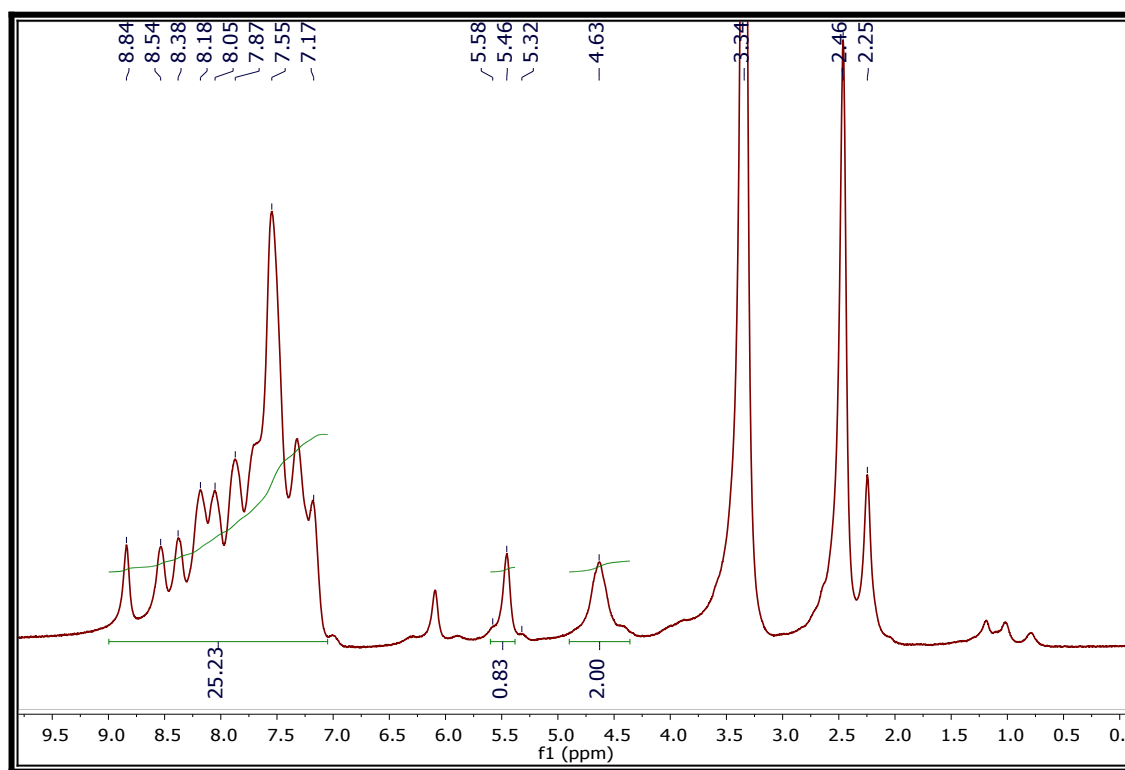
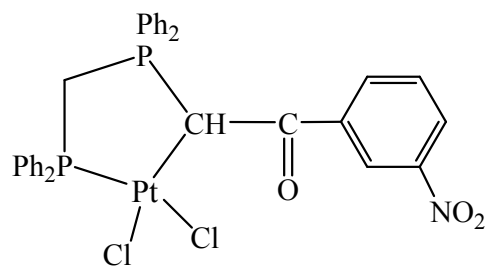


Figure S10. ^1H NMR of $[\text{PtCl}_2(\text{Ph}_2\text{PCH}_2\text{PPh}_2\text{C}(\text{H})\text{C}(\text{O})\text{C}_6\text{H}_4\text{-}m\text{-NO}_2)]$ (**2**).



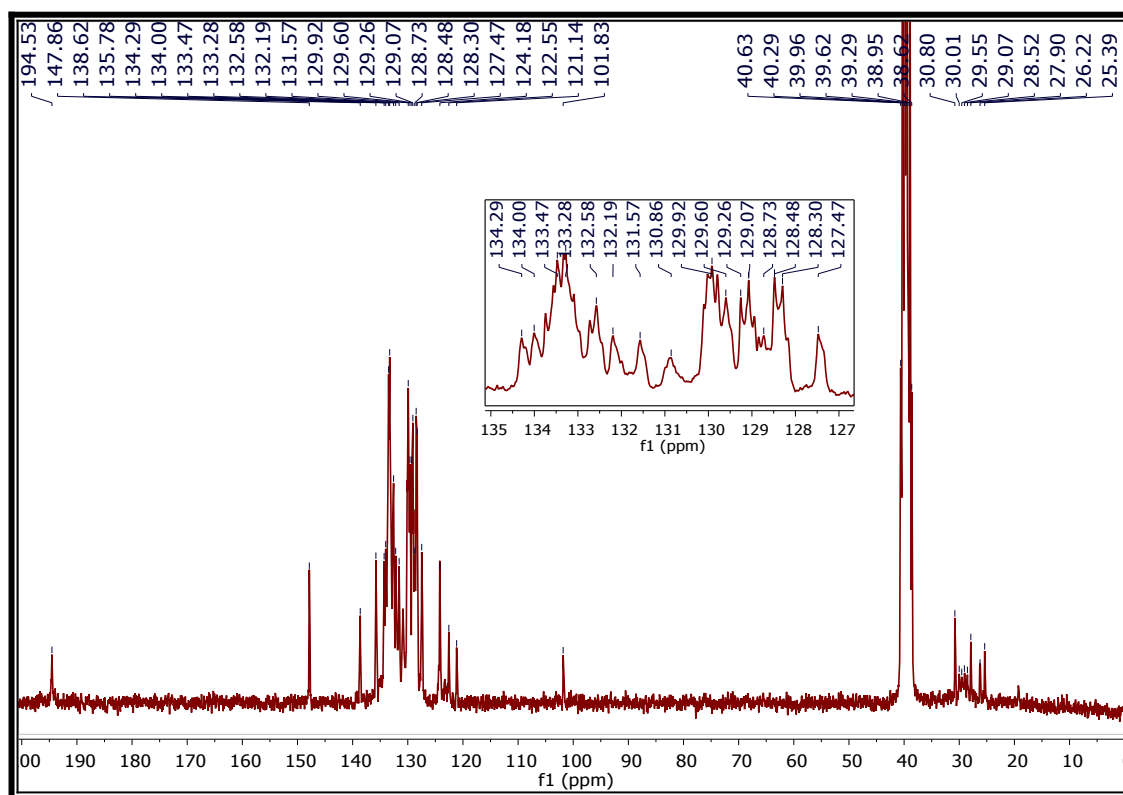
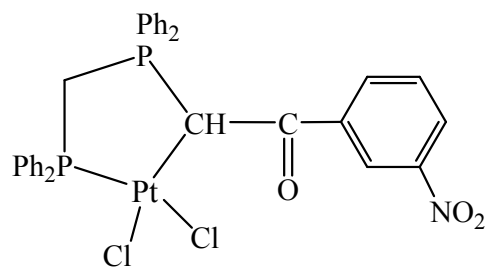


Figure S11. ^{13}C NMR of $[\text{PtCl}_2(\text{Ph}_2\text{PCH}_2\text{PPh}_2\text{C}(\text{H})\text{C}(\text{O})\text{C}_6\text{H}_4\text{-}m\text{-NO}_2)]$ (**2**).



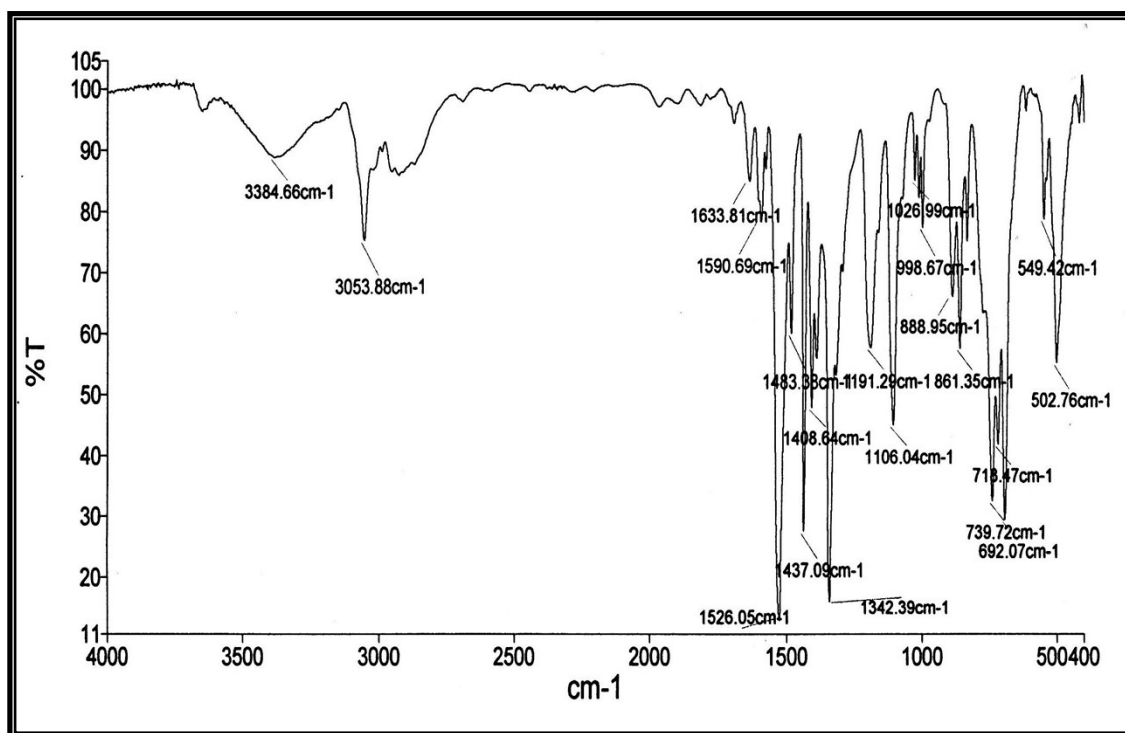
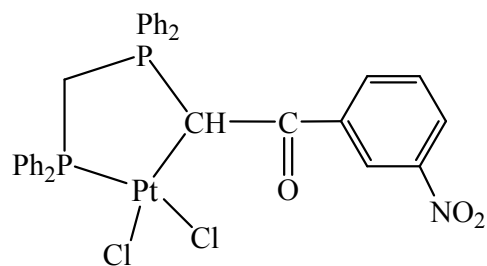


Figure S12. IR spectrum of $[\text{PtCl}_2(\text{Ph}_2\text{PCH}_2\text{PPh}_2\text{C}(\text{H})\text{C}(\text{O})\text{C}_6\text{H}_4\text{-}m\text{-NO}_2)]$ (**2**).



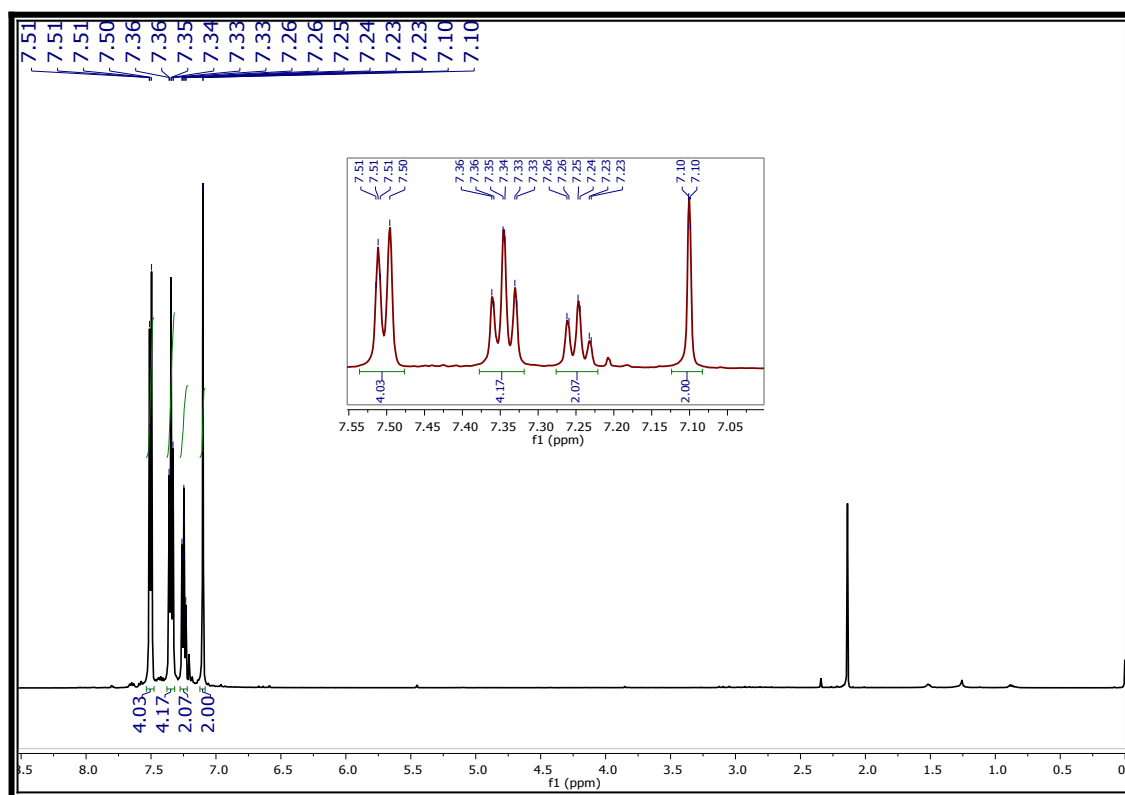
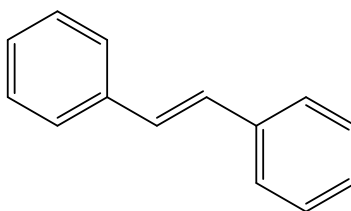


Figure S13. ^1H NMR of (E)-1,2-diphenylethene.



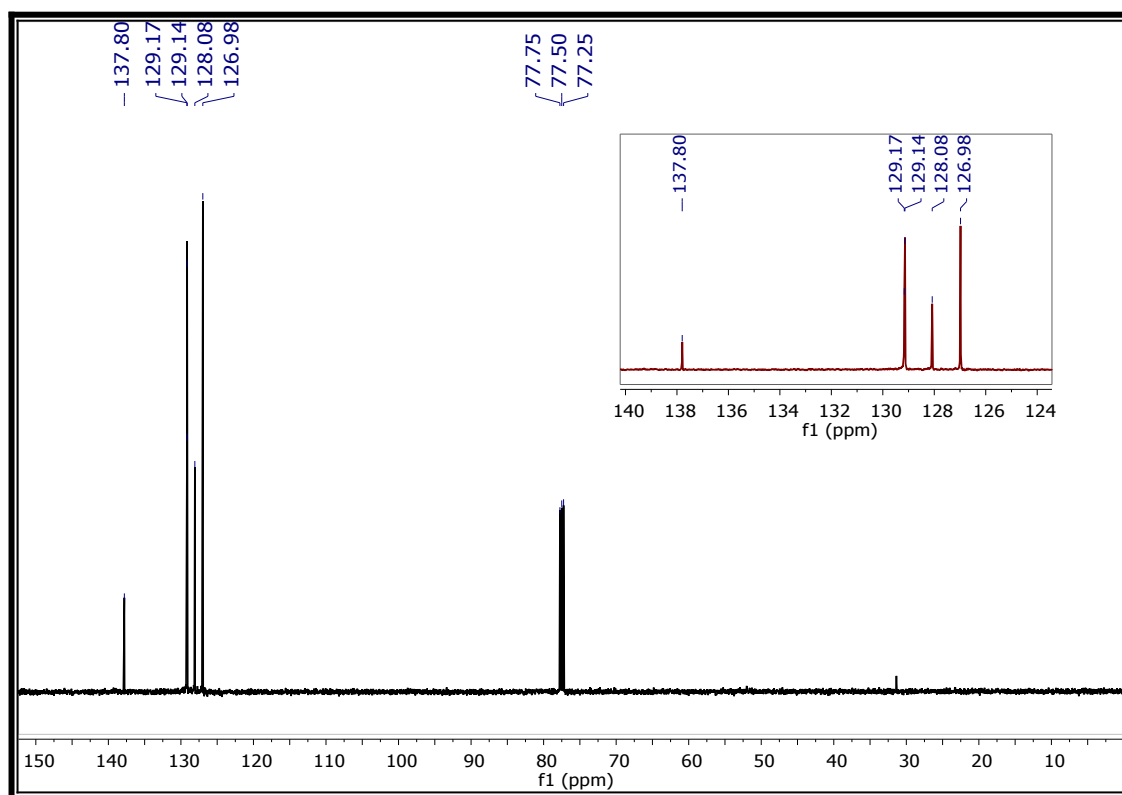
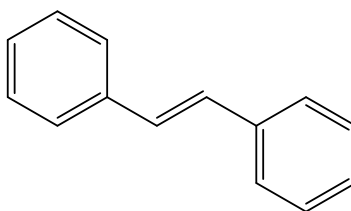


Figure S14. ^{13}C NMR of (E)-1,2-diphenylethene.



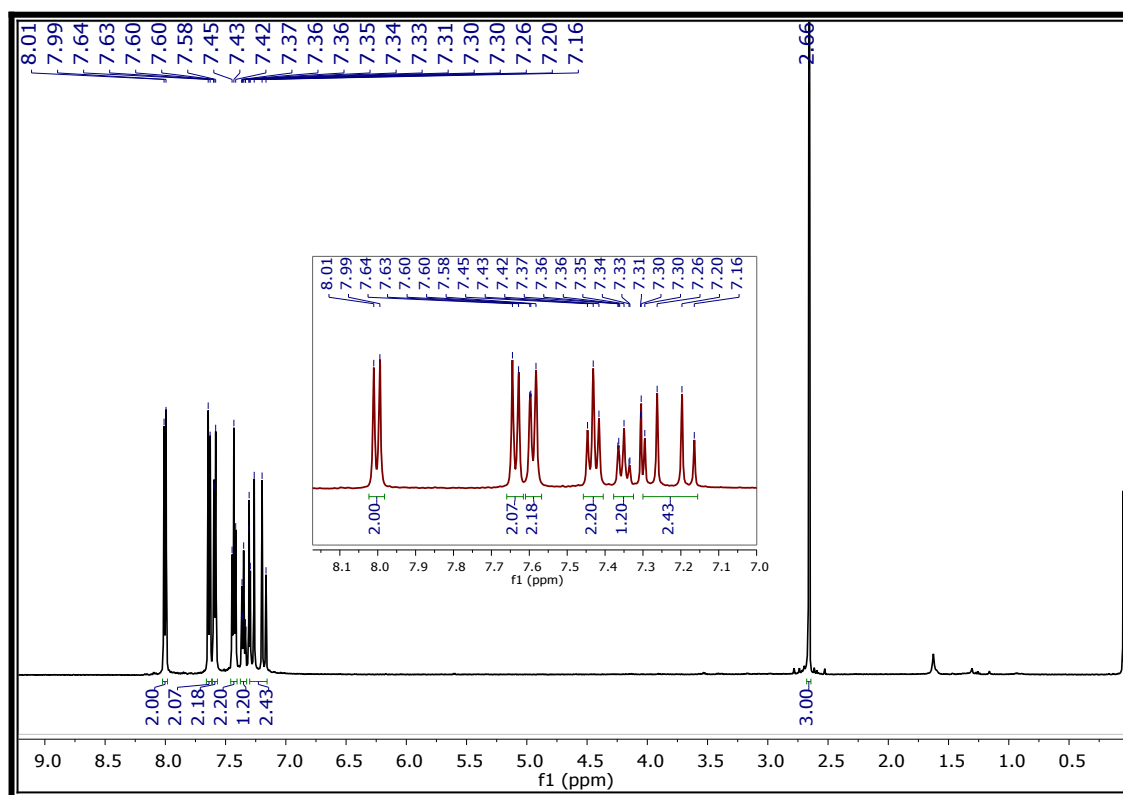
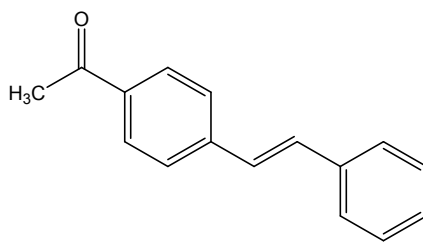


Figure S15. ¹H NMR of (E)-1-(4-styrylphenyl)ethanone.



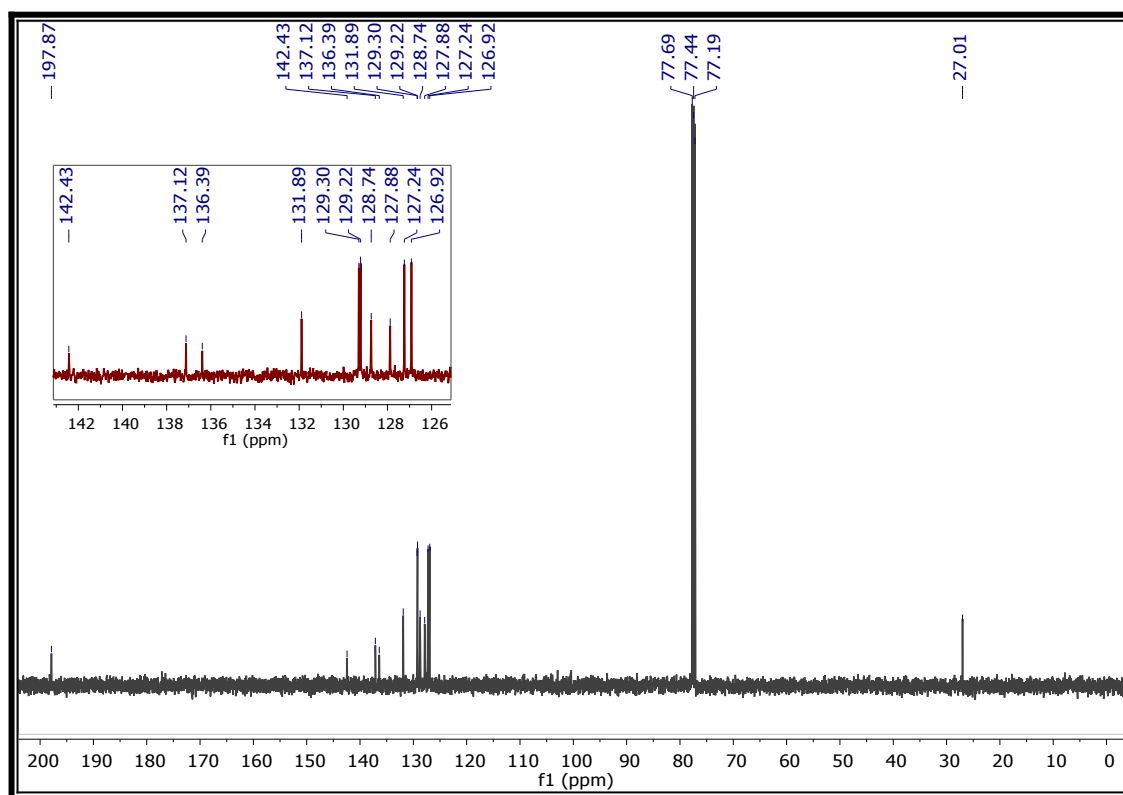
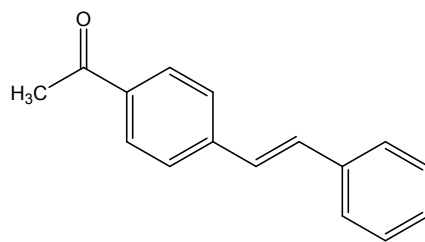


Figure S16. ¹³C NMR of (E)-1-(4-styrylphenyl)ethanone.



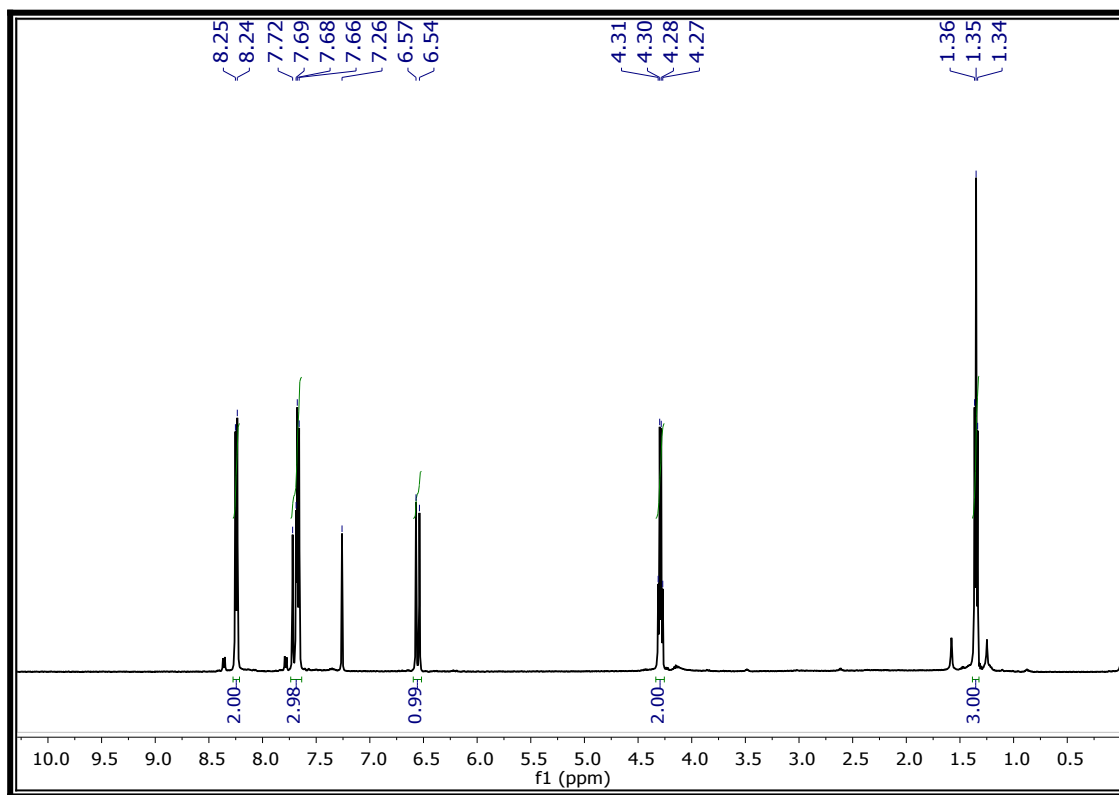
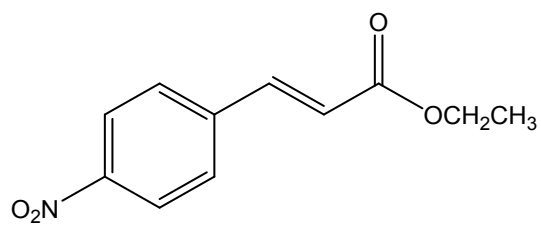


Figure S17. ¹H NMR of (E)-ethyl 3-(4-nitrophenyl)acrylate.



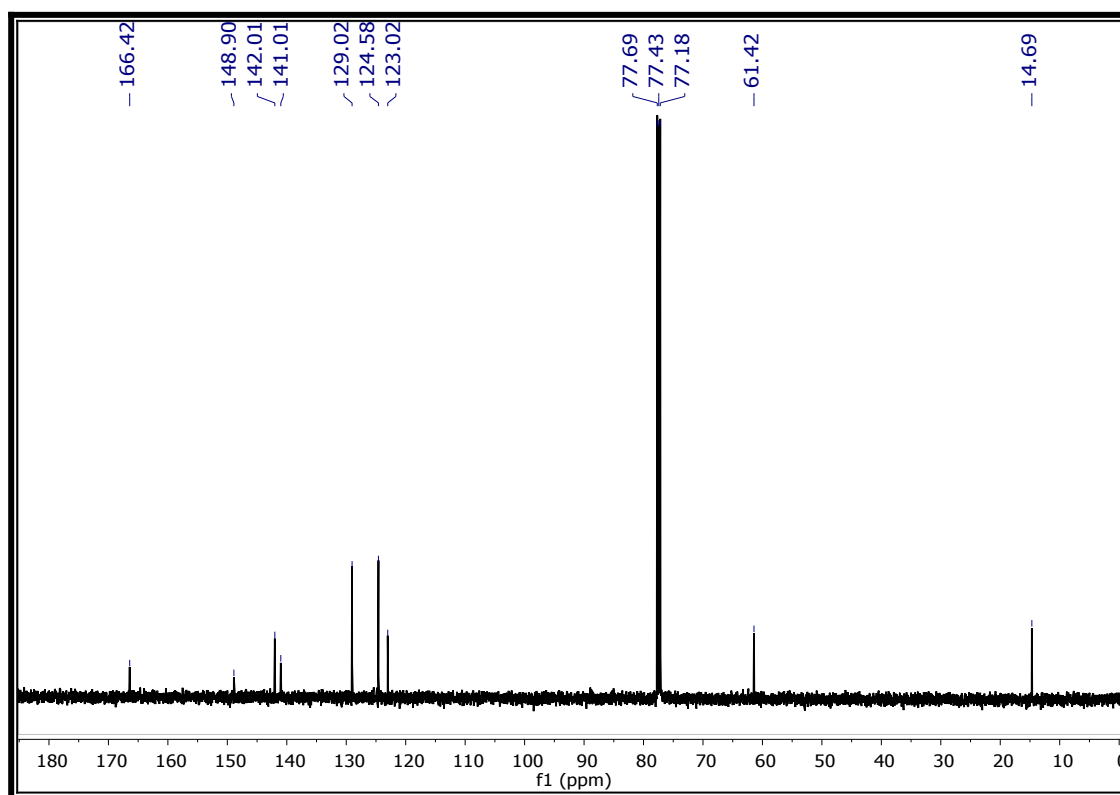


Figure S18. ¹³C NMR of (E)-ethyl 3-(4-nitrophenyl)acrylate.

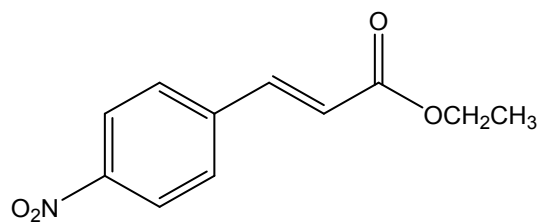


Table S1. Relative electronic energy (E_{elec}), electronic energy corrected with zero point energy (E_{corre}) and Gibbs free energy [kcal/mol] for three isomers of all synthesized derived of Mizoroki-Heck reaction

Products	trans			cis			gem		
	E_{elec}	E_{corre}	Gibbs free	E_{elec}	E_{corre}	Gibbs free	E_{elec}	E_{corre}	Gibbs free
Ph-CH=CH-Ph	0.00	0.00	0.00	5.16	5.38	6.02	10.06	9.61	12.25
NO ₂ -Ph-CH=CH-Ph	0.00	0.00	0.00	5.37	5.53	5.80	16.58	15.73	18.81
CH ₃ -Ph-CH=CH-Ph	0.00	0.00	0.00	5.21	5.46	6.03	5.12	5.13	6.29
CH ₃ O-Ph-CH=CH-Ph	0.00	0.00	0.00	5.12	5.31	5.49	13.41	12.50	15.23
CH ₃ OC-Ph-CH=CH-Ph	0.00	0.00	0.00	5.42	5.63	6.24	5.47	5.41	6.51
CN-Ph-CH=CH-Ph	0.00	0.00	0.00	5.28	5.47	5.80	10.46	9.95	12.37
Ph-CH=CH-EtAcr	0.00	0.00	0.00	5.02	5.31	5.32	7.09	6.81	7.11
NO ₂ -Ph-CH=CH-EtAcr	0.00	0.00	0.00	4.68	4.97	4.84	6.25	6.00	6.26
CH ₃ -Ph-CH=CH-EtAcr	0.00	0.00	0.00	4.91	5.16	4.31	7.43	7.11	7.01
CH ₃ O-Ph-CH=CH-EtAcr	0.00	0.00	0.00	4.59	4.87	4.92	8.03	7.75	7.98
CH ₃ OC-Ph-CH=CH-EtAcr	0.00	0.00	0.00	5.11	5.41	5.37	6.67	6.47	6.85
CN-Ph-CH=CH-EtAcr	0.00	0.00	0.00	4.58	4.88	4.79	6.43	6.17	6.35

Table S1 presents the electronic energy (E_{elec}), the electronic energy corrected for the zero point energy (E_{corre}) and the relative Gibbs free energy (**Gibbs free**) in the gas-phase for the studied isomers of the synthesized derived of Mizoroki-Heck reaction in this study

The cartesian atomic coordinates of studied structures

“YPdCl ₂ complex”							
				C	4.199626000	0.352480000	-1.154590000
				H	4.531587000	0.295256000	-2.202942000
Pd	-0.712282000	-0.640030000	-1.242905000	C	2.836421000	0.535810000	-0.887647000
Cl	0.176257000	0.382971000	-3.216428000	H	2.129899000	0.614184000	-1.732445000
Cl	-1.267824000	-2.586993000	-2.471936000	C	2.371335000	0.567181000	0.447987000
P	-1.505593000	1.946177000	0.532743000	C	3.307214000	0.401080000	1.497364000
P	-1.675854000	-1.674532000	0.531832000	H	2.934293000	0.431214000	2.532379000
O	0.603770000	0.721698000	2.032300000	C	4.665413000	0.221263000	1.224070000
C	6.591939000	0.009964000	-0.403468000	H	5.377863000	0.127516000	2.058838000
C	7.201199000	0.654928000	-1.508380000	C	0.939077000	0.786036000	0.830312000
H	6.598825000	1.321049000	-2.145787000	C	-0.082223000	1.112764000	-0.211850000
C	8.567109000	0.484544000	-1.782217000	H	0.293458000	1.704796000	-1.070938000
H	9.019366000	1.004715000	-2.641778000	C	-1.021068000	3.295253000	1.687907000
C	9.357986000	-0.337860000	-0.960330000	C	-1.018186000	3.124381000	3.088838000
H	10.429662000	-0.473047000	-1.176510000	H	-1.331060000	2.169511000	3.535398000
C	8.768820000	-0.987742000	0.138773000	C	-0.592688000	4.170892000	3.923614000
H	9.376152000	-1.643481000	0.783144000	H	-0.595990000	4.030567000	5.015934000
C	7.403490000	-0.814834000	0.414405000	C	-0.152325000	5.385148000	3.368680000
H	6.949230000	-1.352046000	1.261833000	H	0.184713000	6.201873000	4.026378000
C	5.145156000	0.195539000	-0.111227000	C	-0.138333000	5.553948000	1.972892000

H	0.209249000	6.501509000	1.532251000	N	-5.997266000	-0.593028000	-1.651587000
C	-0.571785000	4.515230000	1.133168000	C	-1.034229000	0.603432000	0.020262000
H	-0.567026000	4.659066000	0.040845000	H	-1.658934000	1.096249000	-0.750307000
C	-2.524589000	2.778417000	-0.741583000	C	-1.802385000	-0.051741000	1.125573000
C	-3.593006000	3.592981000	-0.292290000	C	-3.173092000	-0.618315000	0.860320000
H	-3.765152000	3.747627000	0.785361000	C	-3.906418000	-0.371813000	-0.320318000
C	-4.434890000	4.223405000	-1.220731000	H	-3.491944000	0.178726000	-1.176478000
H	-5.264633000	4.854223000	-0.864808000	C	-5.202989000	-0.891655000	-0.426128000
C	-4.213110000	4.053224000	-2.600117000	C	-5.792021000	-1.670127000	0.581254000
H	-4.873047000	4.550729000	-3.328626000	H	-6.808418000	-2.059066000	0.428593000
C	-3.149843000	3.251123000	-3.044949000	C	-5.055045000	-1.916258000	1.750956000
H	-2.968751000	3.112709000	-4.122332000	H	-5.495445000	-2.521829000	2.558228000
C	-2.302083000	2.605916000	-2.124978000	C	-3.764596000	-1.386298000	1.892194000
H	-1.482883000	1.965653000	-2.503340000	H	-3.177456000	-1.551822000	2.807756000
C	-2.677122000	0.802102000	1.419282000	C	-0.465630000	3.074221000	1.760817000
H	-3.125545000	1.394412000	2.244652000	C	-0.852912000	4.315457000	1.202673000
H	-3.491118000	0.609189000	0.687786000	H	-0.688125000	4.518047000	0.133117000
C	-2.081612000	-0.511448000	1.942578000	C	-1.446251000	5.297616000	2.012279000
H	-2.819499000	-1.016790000	2.600401000	H	-1.743500000	6.260735000	1.568680000
H	-1.149979000	-0.311888000	2.507139000	C	-1.657410000	5.052736000	3.380294000
C	-3.350416000	-2.393411000	0.203562000	H	-2.119746000	5.825810000	4.014109000
C	-4.140923000	-1.880176000	-0.847745000	C	-1.282866000	3.817215000	3.936884000
H	-3.711580000	-1.135814000	-1.536351000	H	-1.455372000	3.616750000	5.005912000
C	-5.452579000	-2.349049000	-1.034967000	C	-0.695432000	2.825778000	3.134417000
H	-6.059952000	-1.947792000	-1.861687000	H	-0.443536000	1.850108000	3.572906000
C	-5.978440000	-3.340729000	-0.188359000	C	1.010164000	2.620982000	-0.737601000
H	-7.002386000	-3.715575000	-0.346030000	C	0.652694000	2.356529000	-2.079751000
C	-5.189701000	-3.863150000	0.851868000	H	-0.104842000	1.594969000	-2.330031000
H	-5.591372000	-4.650180000	1.510001000	C	1.301455000	3.051505000	-3.115760000
C	-3.880974000	-3.390598000	1.050945000	H	1.020596000	2.840461000	-4.159166000
H	-3.265309000	-3.812643000	1.861867000	C	2.302948000	3.993596000	-2.826524000
C	-0.694592000	-3.025686000	1.317863000	H	2.810447000	4.527534000	-3.645531000
C	-0.132233000	-4.016083000	0.478020000	C	2.660719000	4.253955000	-1.491072000
H	-0.290726000	-3.947171000	-0.612481000	H	3.446757000	4.989528000	-1.259396000
C	0.623370000	-5.060159000	1.034300000	C	2.014829000	3.574052000	-0.447158000
H	1.058333000	-5.824869000	0.371356000	H	2.292165000	3.796231000	0.596291000
C	0.834275000	-5.126540000	2.423524000	C	1.452540000	0.773229000	1.570438000
H	1.433028000	-5.944890000	2.854475000	H	1.001047000	0.478083000	2.536048000
C	0.284800000	-4.140872000	3.260237000	H	2.376343000	1.360409000	1.741575000
H	0.450419000	-4.181645000	4.348669000	C	3.452341000	-0.417807000	-0.167456000
C	-0.477023000	-3.092994000	2.713204000	C	4.519452000	-0.109326000	0.709683000
H	-0.891824000	-2.330118000	3.388369000	H	4.367701000	-0.126754000	1.801979000

“Y’PtCl₂ complex”

Pt	0.081870000	-0.922345000	-0.941233000	C	5.788974000	0.202321000	0.196990000
Cl	-1.548163000	-0.850598000	-2.679565000	H	6.615084000	0.437079000	0.887046000
Cl	1.249290000	-2.717970000	-1.992305000	C	6.004119000	0.206025000	-1.193824000
P	0.201301000	1.765635000	0.657573000	H	7.000873000	0.448577000	-1.595881000
P	1.773984000	-0.772804000	0.525256000	C	4.949189000	-0.109365000	-2.066019000
O	-1.322851000	-0.136698000	2.274595000	H	5.115626000	-0.119904000	-3.154783000
O	-5.525467000	0.215975000	-2.451802000	C	3.674361000	-0.422919000	-1.560352000
O	-7.082779000	-1.167323000	-1.775525000	H	2.854215000	-0.712561000	-2.236009000
				C	2.032924000	-2.127729000	1.745208000
				C	1.131860000	-2.292835000	2.821644000
				H	0.294933000	-1.588763000	2.959533000

C	1.279423000	-3.380975000	3.697076000
H	0.577741000	-3.500827000	4.537782000
C	2.305820000	-4.321006000	3.494124000
H	2.415314000	-5.176222000	4.179784000
C	3.181707000	-4.175536000	2.404592000
H	3.974933000	-4.919261000	2.228540000
C	3.047923000	-3.085659000	1.527832000
H	3.725903000	-2.986278000	0.666948000

“1”

Pd	0.592727000	-0.545989000	-0.846271000
P	1.861963000	-1.430144000	0.955500000
C	2.500147000	-0.002021000	1.993306000
C	3.039275000	1.129647000	1.102314000
P	1.786287000	2.251117000	0.300863000
C	0.197251000	1.516290000	0.294446000
H	1.677717000	0.352171000	2.635358000
H	3.306278000	-0.334153000	2.666601000
H	3.658782000	0.715733000	0.292247000
H	3.696575000	1.791720000	1.686526000
H	-0.069507000	0.985663000	1.211555000
C	1.900482000	3.812568000	1.276443000
C	3.124945000	4.488157000	1.426286000
C	0.758674000	4.312792000	1.916984000
C	3.203160000	5.642222000	2.208327000
C	0.839225000	5.469514000	2.698783000
C	2.059021000	6.134250000	2.846414000
H	4.024299000	4.122681000	0.922716000
H	-0.195916000	3.796692000	1.800670000
H	4.159133000	6.160520000	2.317962000
H	-0.057846000	5.852452000	3.191467000
H	2.120243000	7.038317000	3.457604000
C	2.438412000	2.637062000	-1.365566000
C	2.827599000	1.576779000	-2.198999000
C	2.504265000	3.953736000	-1.843605000
C	3.309823000	1.834283000	-3.483944000
C	2.989094000	4.206263000	-3.128956000
C	3.397829000	3.149953000	-3.948358000
H	2.704377000	0.545086000	-1.854346000
H	2.157421000	4.780958000	-1.224002000
H	3.608328000	1.002127000	-4.126342000
H	3.033702000	5.234581000	-3.495916000
H	3.773363000	3.351505000	-4.954918000
C	3.447874000	-2.323150000	0.576224000
C	3.794532000	-2.489492000	-0.773170000
C	4.302158000	-2.843691000	1.563797000
C	4.977614000	-3.145158000	-1.131963000
C	5.482521000	-3.499608000	1.207583000
C	5.824189000	-3.649076000	-0.142007000
H	3.111162000	-2.108431000	-1.536834000
H	4.039870000	-2.751730000	2.621354000
H	5.233700000	-3.266996000	-2.187775000

H	6.136593000	-3.902638000	1.985479000
H	6.747156000	-4.165269000	-0.418987000
C	1.071094000	-2.532357000	2.211083000
C	1.247067000	-2.421615000	3.601470000
C	0.215390000	-3.534017000	1.716377000
C	0.592318000	-3.297487000	4.473967000
C	-0.427801000	-4.415076000	2.588435000
C	-0.242620000	-4.298291000	3.969836000
H	1.897130000	-1.650953000	4.021724000
H	0.046921000	-3.619971000	0.639452000
H	0.737350000	-3.195925000	5.552905000
H	-1.085632000	-5.187688000	2.182737000
H	-0.753433000	-4.981860000	4.653023000
C	-0.824231000	2.287124000	-0.387822000
O	-0.556761000	3.308448000	-1.037508000
C	-2.262270000	1.850477000	-0.253762000
C	-2.650210000	0.586646000	0.220862000
C	-3.266253000	2.763963000	-0.611300000
C	-3.998765000	0.258553000	0.354651000
C	-4.613522000	2.436997000	-0.474590000
C	-5.011159000	1.177973000	0.016605000
H	-1.887190000	-0.157034000	0.460838000
H	-2.957368000	3.734085000	-1.005758000
H	-4.270078000	-0.724572000	0.746188000
H	-5.373816000	3.160916000	-0.777715000
C	-6.448348000	0.829800000	0.170876000
C	-6.911964000	-0.475754000	-0.082657000
C	-7.389217000	1.795145000	0.579019000
C	-8.261070000	-0.803097000	0.066450000
C	-8.738393000	1.468391000	0.729459000
C	-9.181533000	0.167210000	0.473998000
H	-6.209203000	-1.238670000	-0.425256000
H	-7.053897000	2.809911000	0.805331000
H	-8.596731000	-1.821750000	-0.145357000
H	-9.446963000	2.234210000	1.056114000
H	-10.237618000	-0.088928000	0.591016000
C	0.128817000	-1.780766000	-2.660546000
H	1.078998000	-2.036088000	-3.143417000
C	-0.365771000	-0.481179000	-2.831766000
H	-1.429459000	-0.255016000	-2.711842000
H	0.181620000	0.222675000	-3.465590000
C	-0.663407000	-2.956749000	-2.244615000
C	-0.093821000	-4.245548000	-2.322063000
C	-1.990856000	-2.865334000	-1.770855000
C	-0.805074000	-5.384599000	-1.940250000
C	-2.702693000	-4.002972000	-1.391354000
C	-2.117591000	-5.273086000	-1.469640000
H	0.931929000	-4.349398000	-2.688205000
H	-2.469354000	-1.887393000	-1.691391000
H	-0.331354000	-6.367596000	-2.014758000
H	-3.729916000	-3.897997000	-1.030338000
H	-2.679737000	-6.162698000	-1.174281000

“2”

Pd	0.712158000	-0.619441000	-0.818887000
P	2.045956000	-1.466795000	1.003044000
C	2.589495000	-0.030817000	2.081182000
C	3.079683000	1.140653000	1.214305000
P	1.777508000	2.261013000	0.502479000
C	0.232580000	1.441016000	0.378078000
C	1.766528000	3.711401000	1.641999000
C	2.955762000	4.386735000	1.972879000
C	0.561476000	4.124348000	2.228406000
C	2.937208000	5.452533000	2.875046000
C	0.545587000	5.192016000	3.130994000
C	1.730517000	5.856696000	3.456068000
C	2.449769000	2.826827000	-1.100634000
C	2.685899000	1.859400000	-2.088475000
C	2.711174000	4.177006000	-1.375957000
C	3.209388000	2.233648000	-3.326789000
C	3.237998000	4.545975000	-2.615718000
C	3.495141000	3.576244000	-3.589465000
C	3.687073000	-2.230871000	0.597211000
C	4.133982000	-2.157736000	-0.731273000
C	4.496511000	-2.872231000	1.551061000
C	5.372596000	-2.693935000	-1.099242000
C	5.730214000	-3.413630000	1.183370000
C	6.172366000	-3.322460000	-0.141919000
C	1.325598000	-2.655738000	2.216768000
C	1.363918000	-2.493815000	3.613271000
C	0.659146000	-3.777275000	1.688018000
C	0.756156000	-3.432008000	4.455168000
C	0.060232000	-4.716853000	2.529083000
C	0.105437000	-4.545418000	3.916659000
C	-0.806922000	2.243757000	-0.236615000
O	-0.550765000	3.295560000	-0.840975000
C	-2.245016000	1.814525000	-0.079932000
C	-2.643974000	0.589807000	0.479972000
C	-3.244152000	2.712781000	-0.490379000
C	-3.995084000	0.288109000	0.648700000
C	-4.593129000	2.408714000	-0.327695000
C	-5.000730000	1.190897000	0.253315000
C	-6.440601000	0.870045000	0.439006000
C	-6.918185000	-0.446950000	0.293601000
C	-7.371775000	1.874604000	0.767267000
C	-8.270377000	-0.747729000	0.468331000
C	-8.724142000	1.574864000	0.943115000
C	-9.180877000	0.261915000	0.794371000
H	1.742319000	0.269382000	2.718513000
H	3.400799000	-0.343586000	2.757517000
H	3.675886000	0.770708000	0.366062000
H	3.747048000	1.793168000	1.797163000
H	-0.023596000	0.831034000	1.247657000
H	3.906486000	4.091221000	1.520873000
H	-0.367646000	3.609896000	1.979535000

H	3.867599000	5.969082000	3.124005000
H	-0.400356000	5.504681000	3.579818000
H	1.715721000	6.690656000	4.162357000
H	2.409377000	0.815487000	-1.897169000
H	2.486471000	4.945631000	-0.635957000
H	3.372282000	1.473532000	-4.094194000
H	3.435835000	5.600133000	-2.825168000
H	3.902440000	3.869926000	-4.560346000
H	3.487564000	-1.685835000	-1.475687000
H	4.156346000	-2.962279000	2.586231000
H	5.707283000	-2.628276000	-2.137795000
H	6.348398000	-3.915004000	1.932838000
H	7.137175000	-3.749543000	-0.427596000
H	1.868844000	-1.636301000	4.062980000
H	0.592263000	-3.925207000	0.608444000
H	0.794166000	-3.289491000	5.538559000
H	-0.450380000	-5.573581000	2.082794000
H	-0.369566000	-5.275343000	4.577418000
H	-1.893523000	-0.148873000	0.766240000
H	-2.925933000	3.653243000	-0.944400000
H	-4.273515000	-0.660830000	1.112851000
H	-5.347701000	3.117884000	-0.676514000
H	-6.223842000	-1.243066000	0.015651000
H	-7.026562000	2.901070000	0.910170000
H	-8.616302000	-1.776914000	0.340730000
H	-9.424671000	2.372035000	1.205705000
H	-10.239480000	0.027010000	0.931163000
C	-1.409937000	-3.295410000	-1.744225000
C	-0.062737000	-3.159825000	-2.083035000
C	0.461556000	-1.958324000	-2.611197000
C	-0.421845000	-0.844522000	-2.782577000
C	-1.806896000	-0.998265000	-2.476716000
C	-2.281432000	-2.187359000	-1.962425000
Cl	0.017058000	0.434617000	-3.932184000
C	-1.861060000	-4.580646000	-1.149821000
O	-1.059232000	-5.431849000	-0.787672000
C	-3.352978000	-4.819779000	-0.978353000
H	0.589465000	-4.028616000	-1.967217000
H	1.436173000	-1.964091000	-3.104540000
H	-2.481130000	-0.160730000	-2.660743000
H	-3.342508000	-2.262911000	-1.719412000
H	-3.898324000	-4.669519000	-1.923481000
H	-3.507480000	-5.845229000	-0.618838000
H	-3.775513000	-4.115204000	-0.242787000

“3-TS”

Pd	-0.652121000	0.224463000	-0.625956000
P	-1.678452000	1.681471000	0.792032000
C	-2.556620000	0.504516000	1.971657000
C	-3.364049000	-0.583137000	1.241280000
P	-2.456333000	-2.004706000	0.426409000
C	-0.715840000	-1.829449000	0.488884000

C	-3.095308000	-3.484739000	1.331893000	H	-2.684030000	2.397560000	-1.801981000
C	-4.474935000	-3.731102000	1.449544000	H	-3.766793000	3.351638000	2.257754000
C	-2.188937000	-4.360514000	1.944510000	H	-4.592802000	3.785234000	-2.636098000
C	-4.937212000	-4.832001000	2.173849000	H	-5.660470000	4.720367000	1.440723000
C	-2.653779000	-5.463140000	2.668406000	H	-6.084724000	4.946219000	-1.007047000
C	-4.025666000	-5.699875000	2.785441000	H	-0.233514000	1.248993000	3.402791000
C	-3.110098000	-2.158525000	-1.283196000	H	-1.062282000	4.559338000	0.742029000
C	-3.073623000	-1.032102000	-2.119294000	H	1.144514000	2.725634000	4.803906000
C	-3.585814000	-3.377388000	-1.786914000	H	0.346584000	6.025515000	2.136835000
C	-3.537064000	-1.115143000	-3.433624000	H	1.454336000	5.128189000	4.192786000
C	-4.049814000	-3.455849000	-3.102582000	H	1.737542000	-0.762158000	0.580236000
C	-4.032069000	-2.326460000	-3.925980000	H	1.690176000	-4.796582000	-0.879749000
C	-3.104237000	2.762446000	0.275359000	H	4.197820000	-0.853158000	0.801516000
C	-3.351021000	2.904935000	-1.098427000	H	4.179319000	-4.887338000	-0.731553000
C	-3.948692000	3.428683000	1.182082000	H	6.168040000	-0.870567000	-0.444223000
C	-4.416644000	3.684957000	-1.561790000	H	5.943113000	-4.997169000	0.793800000
C	-5.013826000	4.207085000	0.723820000	H	8.632933000	-0.946902000	-0.252491000
C	-5.251281000	4.335369000	-0.650219000	H	8.409983000	-5.083134000	0.954110000
C	-0.777156000	2.792185000	1.967696000	H	9.776474000	-3.056179000	0.440801000
C	-0.130717000	2.298217000	3.116443000	C	2.809244000	4.354911000	-0.884608000
C	-0.585853000	4.147552000	1.634750000	C	1.627335000	4.399586000	-1.647008000
C	0.660642000	3.132581000	3.911681000	C	1.107164000	3.250560000	-2.232163000
C	0.209490000	4.979896000	2.424751000	C	1.776257000	2.035015000	-2.050075000
C	0.834911000	4.476775000	3.570910000	C	2.965916000	1.963545000	-1.323125000
C	0.038196000	-2.834640000	-0.220339000	C	3.473981000	3.126558000	-0.740623000
O	-0.505107000	-3.740448000	-0.876918000	Cl	1.117180000	0.571148000	-2.755531000
C	1.544685000	-2.797334000	-0.124046000	C	3.283681000	5.626460000	-0.241519000
C	2.270440000	-1.681855000	0.326109000	O	2.643344000	6.654463000	-0.358729000
C	2.259447000	-3.944677000	-0.502394000	C	4.568209000	5.599271000	0.566800000
C	3.661182000	-1.725447000	0.419786000	H	1.123797000	5.361831000	-1.757801000
C	3.648926000	-3.987604000	-0.410155000	H	0.182483000	3.281953000	-2.809960000
C	4.383016000	-2.880352000	0.058240000	H	3.472388000	1.004963000	-1.202569000
C	5.865279000	-2.927145000	0.162719000	H	4.396048000	3.058906000	-0.160332000
C	6.652829000	-1.793655000	-0.118314000	H	5.417243000	5.249773000	-0.042313000
C	6.528906000	-4.108840000	0.546748000	H	4.774150000	6.612358000	0.934572000
C	8.044870000	-1.838674000	-0.019418000	H	4.473713000	4.913127000	1.424129000
C	7.920845000	-4.155128000	0.646228000				
C	8.686827000	-3.020120000	0.363732000				
H	-1.794951000	0.045375000	2.619898000				
H	-3.239737000	1.055209000	2.639486000	Pd	0.585549000	-0.276681000	-0.489835000
H	-3.989283000	-0.130102000	0.456024000	P	1.853554000	0.030873000	1.443095000
H	-4.056384000	-1.056865000	1.954159000	C	1.407707000	1.628651000	2.317028000
H	-0.304351000	-1.359116000	1.385028000	C	1.444681000	2.831943000	1.363439000
H	-5.198975000	-3.069270000	0.965875000	P	0.034340000	2.998812000	0.160964000
H	-1.116993000	-4.178312000	1.850667000	C	-0.832642000	1.452962000	0.115871000
H	-6.011526000	-5.014486000	2.258951000	H	0.421761000	1.517140000	2.791804000
H	-1.937885000	-6.141122000	3.139780000	H	2.134020000	1.784823000	3.130164000
H	-4.387079000	-6.562323000	3.351406000	H	2.360186000	2.801978000	0.752774000
H	-2.643933000	-0.095233000	-1.734407000	H	1.494310000	3.770886000	1.934660000
H	-3.574452000	-4.271954000	-1.164164000	H	-1.017276000	1.111270000	1.142185000
H	-3.504464000	-0.231387000	-4.076021000	C	-0.981903000	4.402267000	0.774095000
H	-4.413637000	-4.411006000	-3.489370000	C	-1.097363000	4.652249000	2.152848000
H	-4.393151000	-2.393466000	-4.955631000	C	-1.732510000	5.174935000	-0.129270000

“4”

C	-1.933334000	5.669512000	2.620228000	C	-6.369914000	-2.321936000	-0.084446000
C	-2.563668000	6.192935000	0.343770000	C	-6.131397000	-3.709584000	-0.116154000
C	-2.664910000	6.443945000	1.715354000	C	-7.696499000	-1.884041000	0.094234000
H	-0.539731000	4.055305000	2.878968000	C	-7.177877000	-4.622996000	0.025595000
H	-1.676748000	4.964846000	-1.197530000	C	-8.743129000	-2.797056000	0.237560000
H	-2.011599000	5.856471000	3.694056000	C	-8.489068000	-4.171498000	0.203956000
H	-3.141046000	6.789422000	-0.366786000	H	-5.116157000	-4.076731000	-0.282575000
H	-3.317377000	7.241186000	2.080253000	H	-7.906675000	-0.813147000	0.144433000
C	0.792276000	3.549539000	-1.399625000	H	-6.968292000	-5.695228000	-0.013579000
C	0.742788000	2.765795000	-2.561919000	H	-9.763323000	-2.431923000	0.382864000
C	1.478763000	4.778319000	-1.405968000	H	-9.308346000	-4.886544000	0.314204000
C	1.386204000	3.217165000	-3.719262000	C	1.670512000	-1.954968000	-0.953663000
C	2.116883000	5.217179000	-2.567016000	C	2.516353000	-1.994529000	-2.076577000
C	2.070815000	4.434706000	-3.726429000	C	1.491264000	-3.135126000	-0.218080000
H	0.210371000	1.810650000	-2.584789000	C	3.196028000	-3.160203000	-2.419881000
H	1.510586000	5.404193000	-0.509764000	C	2.156115000	-4.314545000	-0.573137000
H	1.340577000	2.601734000	-4.620918000	C	3.029506000	-4.341888000	-1.672506000
H	2.646730000	6.172960000	-2.566967000	H	2.623149000	-1.110741000	-2.710507000
H	2.567353000	4.779621000	-4.637192000	H	0.824452000	-3.154018000	0.648149000
C	3.661527000	0.295394000	1.201297000	H	3.860179000	-3.191879000	-3.286713000
C	4.152974000	0.463954000	-0.102115000	H	1.984969000	-5.214663000	0.022280000
C	4.549157000	0.410791000	2.287735000	Cl	-0.470853000	-0.551041000	-2.631435000
C	5.506968000	0.742006000	-0.317884000	C	3.783004000	-5.564225000	-2.091454000
C	5.900598000	0.683398000	2.069351000	O	4.562539000	-5.536038000	-3.027244000
C	6.381679000	0.849385000	0.765065000	C	3.557679000	-6.858920000	-1.323447000
H	3.470304000	0.365500000	-0.946923000	H	2.498938000	-7.162166000	-1.360696000
H	4.188589000	0.276685000	3.310939000	H	4.179106000	-7.644807000	-1.771521000
H	5.876464000	0.865826000	-1.338636000	H	3.825944000	-6.742782000	-0.260813000
H	6.582214000	0.764567000	2.919938000				
H	7.440813000	1.059610000	0.595739000			“5”	
C	1.715999000	-1.218545000	2.788354000				
C	0.587745000	-1.226038000	3.628963000	Pd	0.002787000	-0.010819000	-0.107785000
C	2.662080000	-2.249497000	2.921593000	P	0.936474000	1.984008000	-0.797068000
C	0.426813000	-2.218501000	4.598654000	C	2.594121000	1.621294000	-1.584392000
C	2.498296000	-3.241640000	3.892331000	C	3.628835000	0.987859000	-0.644519000
C	1.384505000	-3.227721000	4.736028000	P	3.405374000	-0.797143000	-0.171227000
H	-0.185363000	-0.459988000	3.530510000	C	1.765959000	-1.300303000	-0.641669000
H	3.531224000	-2.283127000	2.262653000	H	2.408189000	0.998717000	-2.472427000
H	-0.45381500						

C	3.663570000	-0.838108000	1.631599000	H	-7.402809000	-1.897593000	-1.653224000
C	2.619496000	-0.477301000	2.500488000	H	-6.946767000	-5.647864000	0.430671000
C	4.929375000	-1.145015000	2.153851000	H	-8.408600000	-3.974346000	-0.704835000
C	2.841031000	-0.433547000	3.876414000	C	-1.765697000	0.872966000	0.412089000
C	5.144212000	-1.095958000	3.534547000	C	-2.126390000	0.675248000	1.755875000
C	4.103107000	-0.743058000	4.395804000	C	-2.692546000	1.442873000	-0.465992000
H	1.629973000	-0.241179000	2.101296000	C	-3.397516000	1.033293000	2.206917000
H	5.749073000	-1.432256000	1.492592000	C	-3.968197000	1.801549000	-0.011329000
H	2.022854000	-0.163438000	4.547975000	C	-4.334912000	1.603346000	1.329334000
H	6.130357000	-1.340586000	3.935677000	H	-1.424573000	0.229755000	2.469677000
H	4.272540000	-0.711615000	5.474650000	H	-2.439186000	1.614161000	-1.515101000
C	1.308510000	3.260430000	0.461932000	H	-3.693386000	0.882365000	3.247559000
C	0.774639000	3.136161000	1.754653000	H	-4.674532000	2.241847000	-0.718795000
C	2.126860000	4.366574000	0.158651000	C	-5.685364000	1.974531000	1.884800000
C	1.050751000	4.101408000	2.727815000	O	-5.933887000	1.789519000	3.059425000
C	2.403867000	5.324365000	1.135292000	C	-6.717654000	2.578447000	0.951825000
C	1.866214000	5.192937000	2.421033000	H	-6.948526000	1.892310000	0.120881000
H	0.127667000	2.291155000	1.993430000	H	-7.633169000	2.780558000	1.521614000
H	2.541550000	4.497813000	-0.843838000	H	-6.349210000	3.517739000	0.508291000
H	0.623380000	3.998647000	3.727863000				
H	3.037972000	6.179819000	0.890669000				
H	2.082689000	5.946161000	3.182370000				
C	0.033325000	2.813307000	-2.160186000	Pd	-0.535464000	-0.334936000	-0.027221000
C	-0.153619000	2.116344000	-3.368883000	P	-1.707403000	0.475373000	-1.921787000
C	-0.522957000	4.094199000	-2.015719000	C	-0.716516000	1.797820000	-2.790904000
C	-0.857064000	2.702970000	-4.422066000	C	-0.464215000	3.057456000	-1.953668000
C	-1.232167000	4.675179000	-3.071824000	P	0.516946000	2.858001000	-0.384451000
C	-1.396944000	3.985657000	-4.275536000	C	1.196335000	1.206541000	-0.390910000
H	0.243448000	1.104963000	-3.493553000	C	1.800006000	4.159162000	-0.410096000
H	-0.408544000	4.643616000	-1.079937000	C	2.518012000	4.410215000	-1.593710000
H	-0.988553000	2.155374000	-5.358317000	C	2.150545000	4.838002000	0.768495000
H	-1.657969000	5.673833000	-2.949063000	C	3.551969000	5.347872000	-1.602948000
H	-1.949734000	4.443911000	-5.098956000	C	3.185669000	5.776067000	0.751979000
C	1.196482000	-2.466395000	0.069619000	C	3.883749000	6.034851000	-0.430595000
O	1.813172000	-3.126338000	0.898444000	C	-0.610903000	3.253833000	0.990917000
C	-0.289401000	-2.659982000	-0.103929000	C	-0.778970000	2.382986000	2.076101000
C	-1.014216000	-2.233142000	-1.243780000	C	-1.326570000	4.464441000	0.952639000
C	-0.995275000	-3.329006000	0.920272000	C	-1.674326000	2.705996000	3.099913000
C	-2.388752000	-2.466726000	-1.340839000	C	-2.213702000	4.786098000	1.981535000
C	-2.362898000	-3.536414000	0.822468000	C	-2.392203000	3.904500000	3.053558000
C	-3.095908000	-3.109774000	-0.310879000	C	-3.322906000	1.315737000	-1.693670000
H	-0.497699000	-1.809058000	-2.107334000	C	-3.751711000	1.660850000	-0.403262000
H	-0.434310000	-3.673828000	1.790920000	C	-4.104290000	1.694709000	-2.802799000
H	-2.912880000	-2.170959000	-2.251187000	C	-4.945316000	2.366082000	-0.220493000
H	-2.887162000	-4.025040000	1.646076000	C	-5.296587000	2.395784000	-2.615446000
C	-4.556721000	-3.345669000	-0.414541000	C	-5.719738000	2.730788000	-1.323830000
C	-5.394198000	-2.413492000	-1.058003000	C	-1.944677000	-0.775617000	-3.244001000
C	-5.141487000	-4.508514000	0.123423000	C	-0.854321000	-1.165590000	-4.043383000
C	-6.767891000	-2.637238000	-1.159259000	C	-3.184084000	-1.412317000	-3.427025000
C	-6.514609000	-4.733739000	0.016654000	C	-1.008993000	-2.149005000	-5.023379000
C	-7.333251000	-3.798754000	-0.623972000	C	-3.334740000	-2.393690000	-4.410276000
H	-4.970077000	-1.488536000	-1.455326000	C	-2.251154000	-2.762230000	-5.212272000
H	-4.513082000	-5.260817000	0.605268000	C	2.298536000	1.067560000	0.574586000

“6”

O	2.278288000	1.706257000	1.633617000	H	7.705444000	-5.461943000	-1.718147000
C	3.442047000	0.142665000	0.282776000	H	10.251773000	-2.532502000	0.166442000
C	3.547074000	-0.644067000	-0.879579000	H	9.972989000	-4.738756000	-0.966648000
C	4.486368000	0.073114000	1.223016000	H	-3.055320000	-0.495867000	1.760643000
C	4.648870000	-1.470349000	-1.088633000	H	-1.430320000	-3.049997000	-1.340987000
C	5.586824000	-0.751048000	1.012749000	H	-4.863369000	-2.150655000	2.143020000
C	5.695779000	-1.544752000	-0.147682000	H	-3.198443000	-4.692608000	-0.908617000
C	6.871119000	-2.423690000	-0.373158000	H	-4.463029000	-6.387967000	0.309630000
C	6.732449000	-3.668522000	-1.017298000	H	-6.243080000	-6.349280000	0.529705000
C	8.156180000	-2.034663000	0.052157000	H	-5.479871000	-5.585990000	-0.903536000
C	7.837673000	-4.494844000	-1.226713000	C	0.708999000	-2.068728000	1.127129000
C	9.262040000	-2.858820000	-0.162290000	C	0.644073000	-1.270715000	2.235040000
C	9.107442000	-4.092708000	-0.801438000	C	-0.193689000	-1.440421000	3.426923000
C	-2.109550000	-1.642994000	0.169075000	C	-1.097589000	-2.509521000	3.595305000
C	-3.081881000	-1.403378000	1.151766000	C	-1.834060000	-2.636532000	4.771501000
C	-2.171476000	-2.833676000	-0.566842000	C	-1.682734000	-1.703103000	5.804603000
C	-4.099513000	-2.330454000	1.383256000	C	-0.784196000	-0.641296000	5.657897000
C	-3.183311000	-3.769891000	-0.324418000	C	-0.046786000	-0.512407000	4.480208000
C	-4.164408000	-3.527156000	0.651075000	H	0.109986000	-2.975558000	1.035711000
C	-5.285168000	-4.485136000	0.958616000	H	1.538609000	-1.954159000	0.426025000
O	-6.098770000	-4.216714000	1.820393000	H	1.369708000	-0.457079000	2.317689000
C	-5.373525000	-5.781488000	0.175890000	H	-1.222499000	-3.250724000	2.804727000
H	0.230095000	1.351702000	-3.128171000	H	-2.529405000	-3.471133000	4.887213000
H	-1.269981000	2.082743000	-3.700030000	H	-2.258598000	-1.810875000	6.726989000
H	-1.419970000	3.521884000	-1.668758000	H	-0.649667000	0.079900000	6.467719000
H	0.065968000	3.798553000	-2.569275000	H	0.668259000	0.308212000	4.372419000
H	1.465820000	0.956446000	-1.423091000				
H	2.285453000	3.874288000	-2.517891000				
H	1.623845000	4.629219000	1.700259000				
H	4.100488000	5.541073000	-2.527670000	Pd	-0.648127000	-0.081419000	0.480955000
H	3.450465000	6.302525000	1.671758000	P	-1.869553000	-0.194502000	-1.727055000
H	4.692069000	6.769875000	-0.439111000	C	-1.349991000	1.217909000	-2.835030000
H	-0.192117000	1.468149000	2.131287000	C	-1.339160000	2.545691000	-2.066964000
H	-1.191196000	5.169278000	0.127878000	P	0.115359000	2.864508000	-0.966341000
H	-1.797802000	2.019830000	3.940760000	C	0.811310000	1.271482000	-0.462015000
H	-2.763990000	5.729121000	1.947072000	C	1.335412000	3.810689000	-1.946125000
H	-3.085827000	4.158304000	3.858869000	C	1.293134000	3.798123000	-3.352784000
H	-3.148739000	1.382242000	0.460861000	C	2.369296000	4.510913000	-1.293511000
H	-3.792023000	1.433732000	-3.816958000	C	2.263469000	4.477633000	-4.093214000
H	-5.269858000	2.625841000	0.789579000	C	3.331381000	5.191082000	-2.042468000
H	-5.899637000	2.679578000	-3.481238000	C	3.282037000	5.176280000	-3.439751000
H	-6.655663000	3.276087000	-1.180275000	C	-0.551483000	3.941144000	0.334702000
H	0.129503000	-0.709418000	-3.910535000	C	-1.179760000	3.378025000	1.454730000
H	-4.038107000	-1.145367000	-2.802608000	C	-0.574696000	5.334081000	0.144977000
H	-0.155119000	-2.435256000	-5.641967000	C	-1.824336000	4.200789000	2.380219000
H	-4.306861000	-2.873234000	-4.547292000	C	-1.221168000	6.150382000	1.076141000
H	-2.372751000	-3.528187000	-5.981815000	C	-1.847353000	5.585886000	2.191453000
H	2.765031000	-0.618636000	-1.641350000	C	-3.694337000	0.027120000	-1.641690000
H	4.408612000	0.682569000	2.125016000	C	-4.238001000	0.649645000	-0.504270000
H	4.713568000	-2.049939000	-2.011681000	C	-4.553638000	-0.379038000	-2.677708000
H	6.369374000	-0.800012000	1.772619000	C	-5.614444000	0.875940000	-0.409226000
H	5.743159000	-4.008068000	-1.332871000	C	-5.928841000	-0.158919000	-2.575655000
H	8.297394000	-1.063748000	0.532389000	C	-6.460609000	0.469281000	-1.444082000

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C	-1.610258000	-1.687096000	-2.769346000	H	-1.055765000	-4.981817000	-4.801716000
C	-0.984365000	-1.656536000	-4.028254000	H	2.009293000	-1.081411000	-0.944281000
C	-2.029139000	-2.928733000	-2.253893000	H	4.498304000	1.575429000	1.364802000
C	-0.784737000	-2.837134000	-4.751781000	H	3.832841000	-2.711272000	-1.055718000
C	-1.834647000	-4.102847000	-2.982201000	H	6.331579000	-0.095844000	1.301138000
C	-1.209379000	-4.061757000	-4.232925000	H	5.015074000	-4.261393000	0.148186000
C	2.078355000	1.445154000	0.290728000	H	7.916779000	-1.065164000	-0.044957000
O	2.265224000	2.457520000	0.968226000	H	6.842356000	-5.922466000	0.042432000
C	3.130053000	0.383284000	0.210014000	H	9.740697000	-2.730731000	-0.124067000
C	2.957642000	-0.843233000	-0.458954000	H	9.218852000	-5.171234000	-0.087852000
C	4.365747000	0.630344000	0.835347000	H	-2.096857000	-0.749874000	1.864918000
C	3.986628000	-1.780331000	-0.506445000	H	-0.011762000	-4.520608000	2.231401000
C	5.391817000	-0.307354000	0.787143000	H	-4.113571000	-1.964081000	1.052851000
C	5.229319000	-1.535722000	0.113534000	H	-2.073121000	-5.711963000	1.616749000
C	6.325679000	-2.535555000	0.058139000	H	-4.438019000	-6.435044000	2.004104000
C	6.048718000	-3.916567000	0.070166000	H	-5.652564000	-6.390097000	0.682156000
C	7.672678000	-2.129163000	-0.008011000	H	-3.906949000	-6.571830000	0.317084000
C	7.079722000	-4.855951000	0.020396000	C	0.409250000	-1.838289000	2.465016000
C	8.703359000	-3.068765000	-0.062709000	C	0.441735000	-0.308063000	2.347724000
C	8.411572000	-4.436042000	-0.047538000	C	-0.076752000	0.482924000	3.493511000
C	-0.868018000	-2.543937000	2.043788000	C	-1.101747000	0.026462000	4.354790000
C	-2.040723000	-1.841893000	1.703034000	C	-1.503772000	0.774151000	5.462618000
C	-0.908546000	-3.947230000	1.981297000	C	-0.891403000	1.998811000	5.750315000
C	-3.207216000	-2.511330000	1.319901000	C	0.130907000	2.465479000	4.916697000
C	-2.077106000	-4.620168000	1.628135000	C	0.532057000	1.721456000	3.807628000
C	-3.245041000	-3.911252000	1.289128000	H	0.645292000	-2.134218000	3.506373000
C	-4.539239000	-4.576164000	0.890220000	H	1.231150000	-2.249681000	1.856395000
O	-5.472696000	-3.899184000	0.508462000	H	1.457576000	0.017371000	2.119755000
C	-4.641593000	-6.084798000	0.979176000	H	-1.581101000	-0.937550000	4.178202000
H	-0.359687000	0.990201000	-3.257461000	H	-2.291035000	0.389187000	6.115811000
H	-2.052753000	1.282672000	-3.680343000	H	-1.197566000	2.575444000	6.626623000
H	-2.225215000	2.626930000	-1.418881000	H	0.629632000	3.412187000	5.139123000
H	-1.396221000	3.405357000	-2.752092000	H	1.338447000	2.094812000	3.172451000
H	0.960200000	0.705901000	-1.391640000				
H	0.507204000	3.264227000	-3.890157000				
H	2.425255000	4.511004000	-0.204774000				
H	2.218709000	4.462970000	-5.184573000	Pd	-0.601807000	-0.191986000	0.644920000
H	4.126526000	5.735147000	-1.527514000	P	-2.057116000	-0.507900000	-1.389649000
H	4.037895000	5.710389000	-4.020397000	C	-1.549733000	0.645381000	-2.774143000
H	-1.144813000	2.298229000	1.608720000	C	-1.523358000	2.104009000	-2.305160000
H	-0.091591000	5.787395000	-0.722379000	P	-0.111507000	2.641572000	-1.228944000
H	-2.294401000	3.754134000	3.258560000	C	0.691977000	1.178028000	-0.539373000
H	-1.233763000	7.232574000	0.927603000	C	1.052654000	3.558340000	-2.298914000
H	-2.350305000	6.228300000	2.918241000	C	1.141759000	3.259864000	-3.671215000
H	-3.579883000	0.953165000	0.314720000	C	1.926705000	4.510087000	-1.740414000
H	-4.151487000	-0.879397000	-3.561974000	C	2.080796000	3.911807000	-4.473674000
H	-6.026334000	1.360548000	0.479147000	C	2.858934000	5.160452000	-2.551553000
H	-6.590646000	-0.485044000	-3.381542000	C	2.937936000	4.864523000	-3.915694000
H	-7.537826000	0.634188000	-1.366449000	C	-0.861622000	3.810134000	-0.061556000
H	-0.650475000	-0.716842000	-4.470285000	C	-1.277728000	3.379590000	1.204932000
H	-2.519153000	-2.979300000	-1.279697000	C	-1.147527000	5.120376000	-0.486332000
H	-0.299761000	-2.793835000	-5.729973000	C	-1.973676000	4.252740000	2.044170000
H	-2.173164000	-5.056356000	-2.570019000	C	-1.844850000	5.986775000	0.358053000

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C	-2.259346000	5.554118000	1.621954000	H	-5.841143000	1.240817000	1.287026000
C	-3.821384000	-0.040971000	-1.161141000	H	-6.807186000	0.256743000	-2.803317000
C	-4.223905000	0.448697000	0.092839000	H	-7.504272000	1.111052000	-0.567273000
C	-4.764985000	-0.098896000	-2.204203000	H	0.041914000	-1.934110000	-2.840044000
C	-5.542273000	0.863132000	0.306405000	H	-4.086022000	-2.710704000	-1.763053000
C	-6.081350000	0.312604000	-1.988504000	H	0.146387000	-4.111900000	-3.986247000
C	-6.472419000	0.792314000	-0.732986000	H	-3.968644000	-4.877570000	-2.927073000
C	-2.044639000	-2.138682000	-2.244669000	H	-1.858553000	-5.598718000	-4.053644000
C	-0.851142000	-2.565494000	-2.859243000	H	2.076413000	-1.120724000	-0.773058000
C	-3.158477000	-2.994022000	-2.262220000	H	4.423044000	2.038452000	0.980994000
C	-0.784441000	-3.801064000	-3.505647000	H	4.058897000	-2.562020000	-0.857314000
C	-3.087830000	-4.230927000	-2.912608000	H	6.420662000	0.564100000	0.953650000
C	-1.906808000	-4.635503000	-3.539967000	H	5.498137000	-3.822457000	0.409895000
C	1.965608000	1.541237000	0.126596000	H	7.995003000	-0.394267000	-0.418790000
O	2.083247000	2.633489000	0.685499000	H	7.487421000	-5.286995000	0.328068000
C	3.114468000	0.581250000	0.093966000	H	9.983622000	-1.860374000	-0.473596000
C	3.029048000	-0.730218000	-0.409551000	H	9.745688000	-4.318012000	-0.107886000
C	4.357326000	1.025686000	0.579663000	H	-2.047225000	-0.965874000	2.541950000
C	4.148441000	-1.558192000	-0.437152000	H	0.724530000	-4.126334000	1.524983000
C	5.474411000	0.197255000	0.551015000	H	-3.902164000	-2.302839000	1.558115000
C	5.399541000	-1.114145000	0.038364000	H	-1.148812000	-5.504819000	0.731230000
C	6.593650000	-1.995905000	-0.000605000	H	-3.289472000	-6.769921000	1.268584000
C	6.476528000	-3.385652000	0.196685000	H	-4.667559000	-6.695016000	0.116412000
C	7.876571000	-1.464810000	-0.237162000	H	-2.985955000	-6.453056000	-0.451769000
C	7.600051000	-4.212943000	0.160709000	C	0.663394000	-1.659074000	2.681696000
C	8.999375000	-2.292919000	-0.277995000	C	0.619105000	-0.147630000	2.445011000
C	8.866252000	-3.670285000	-0.078161000	C	0.091481000	0.714874000	3.529547000
C	-0.497924000	-2.423753000	2.061524000	C	-0.822182000	0.261938000	4.510376000
C	-1.819016000	-1.917058000	2.053841000	C	-1.238645000	1.090458000	5.553638000
C	-0.288660000	-3.716370000	1.540448000	C	-0.749933000	2.396769000	5.657445000
C	-2.881339000	-2.690179000	1.559345000	C	0.165611000	2.862348000	4.706575000
C	-1.350202000	-4.494078000	1.091128000	C	0.579497000	2.037719000	3.661345000
C	-2.665419000	-3.988354000	1.090032000	H	0.711505000	-1.891421000	3.762960000
C	-3.853680000	-4.779271000	0.606606000	H	1.593448000	-2.056625000	2.249537000
O	-4.914983000	-4.219247000	0.410216000	H	1.588589000	0.224138000	2.111279000
C	-3.691205000	-6.266338000	0.374905000	H	-1.197659000	-0.762368000	4.484261000
H	-0.577926000	0.316576000	-3.173061000	H	-1.937258000	0.706424000	6.301312000
H	-2.274049000	0.539818000	-3.596791000	H	-1.065419000	3.039264000	6.483087000
H	-2.432447000	2.329686000	-1.726883000	H	0.571916000	3.873750000	4.787134000
H	-1.535715000	2.794913000	-3.161786000	H	1.303991000	2.412361000	2.935027000
H	0.844171000	0.499723000	-1.389528000				
H	0.484638000	2.518787000	-4.131713000				
H	1.885830000	4.730918000	-0.673510000				
H	2.139414000	3.675506000	-5.538585000	Pd	-0.964676000	-0.659781000	0.530346000
H	3.529819000	5.901690000	-2.111253000	P	-2.447310000	-1.295394000	-1.182341000
H	3.669260000	5.376559000	-4.545562000	C	-2.412109000	-0.019274000	-2.541136000
H	-1.039401000	2.369016000	1.537818000	C	-2.856920000	1.384419000	-2.110943000
H	-0.826033000	5.472169000	-1.468974000	P	-1.879243000	2.256211000	-0.783643000
H	-2.278495000	3.913379000	3.036208000	C	-0.397878000	1.309356000	-0.473042000
H	-2.062065000	7.004908000	0.026929000	C	-1.522025000	3.929900000	-1.430052000
H	-2.801497000	6.236437000	2.281068000	C	-1.111041000	4.096621000	-2.765027000
H	-3.495937000	0.510015000	0.905218000	C	-1.541767000	5.039704000	-0.569035000
H	-4.479571000	-0.477387000	-3.189003000	C	-0.751423000	5.360072000	-3.237357000

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C	-1.180641000	6.301198000	-1.048242000	H	-7.992221000	-1.396767000	0.292483000
C	-0.789543000	6.464374000	-2.379915000	H	-0.633453000	-2.025308000	-3.429634000
C	-3.021094000	2.474719000	0.621407000	H	-3.523845000	-4.035451000	-0.898581000
C	-2.677473000	2.100805000	1.927948000	H	-0.141828000	-4.158364000	-4.551245000
C	-4.278777000	3.054318000	0.370331000	H	-3.002803000	-6.171815000	-2.025223000
C	-3.594030000	2.288775000	2.966643000	H	-1.314356000	-6.249893000	-3.860912000
C	-5.187301000	3.241483000	1.413010000	H	1.981349000	0.151158000	-1.170333000
C	-4.845863000	2.855882000	2.713779000	H	2.467584000	3.525445000	1.463145000
C	-4.224387000	-1.363898000	-0.718345000	H	4.403620000	0.036623000	-1.495123000
C	-4.612502000	-1.025522000	0.587516000	H	4.924216000	3.399436000	1.162941000
C	-5.211630000	-1.712787000	-1.660051000	H	6.440848000	-0.446990000	-0.851302000
C	-5.963784000	-1.036478000	0.949065000	H	6.614887000	3.822470000	-0.145195000
C	-6.558922000	-1.722619000	-1.295489000	H	8.862054000	-0.471955000	-1.246662000
C	-6.936759000	-1.385367000	0.009891000	H	9.050782000	3.777792000	-0.520665000
C	-2.126328000	-2.865438000	-2.081417000	H	10.200435000	1.631735000	-1.078125000
C	-1.168394000	-2.922774000	-3.110984000	C	1.016194000	-3.620113000	0.979402000
C	-2.775757000	-4.052016000	-1.694176000	C	1.471008000	-3.153616000	-0.266953000
C	-0.882200000	-4.132998000	-3.748192000	C	1.968434000	-4.013340000	1.930497000
C	-2.484289000	-5.260549000	-2.332824000	C	2.831281000	-3.045658000	-0.535447000
C	-1.539012000	-5.304653000	-3.361522000	C	3.335952000	-3.921153000	1.659170000
C	0.568350000	2.071753000	0.346566000	C	3.784886000	-3.418532000	0.428135000
O	0.159621000	2.906418000	1.159984000	C	5.238444000	-3.232440000	0.095019000
C	2.040740000	1.870763000	0.159065000	O	5.556555000	-2.621658000	-0.910544000
C	2.613355000	0.882215000	-0.661703000	C	6.285123000	-3.796201000	1.032406000
C	2.906690000	2.765528000	0.814347000	C	-0.463294000	-3.689732000	1.280642000
C	3.993774000	0.809811000	-0.843152000	C	-1.190026000	-2.424819000	1.741145000
C	4.282847000	2.694888000	0.630193000	C	-0.663721000	-1.471828000	2.712764000
C	4.863624000	1.727480000	-0.217861000	C	-1.468443000	-0.996737000	3.791276000
C	6.331307000	1.691918000	-0.452126000	C	-1.017295000	0.007566000	4.629150000
C	6.993167000	0.491578000	-0.780122000	C	0.228822000	0.630071000	4.399394000
C	7.101179000	2.869500000	-0.363573000	C	1.018986000	0.219462000	3.336674000
C	8.371932000	0.473231000	-1.000033000	C	0.592818000	-0.825393000	2.491482000
C	8.478484000	2.849076000	-0.586608000	H	0.742247000	-2.883637000	-1.034560000
C	9.121807000	1.648963000	-0.903499000	H	1.637650000	-4.394113000	2.900576000
H	-1.390337000	0.000988000	-2.947894000	H	3.191031000	-2.677626000	-1.498068000
H	-3.068757000	-0.361567000	-3.357045000	H	4.049583000	-4.233394000	2.423826000
H	-3.896767000	1.354862000	-1.753625000	H	6.121361000	-4.869498000	1.218136000
H	-2.854170000	2.044282000	-2.990583000	H	7.278473000	-3.644422000	0.592220000
H	-0.004081000	0.966985000	-1.438722000	H	6.244809000	-3.285315000	2.008726000
H	-1.058810000	3.245250000	-3.449054000	H	-0.625577000	-4.443595000	2.073585000
H	-1.827946000	4.917570000	0.476127000	H	-0.992681000	-4.076461000	0.395209000
H	-0.438526000	5.481371000	-4.276941000	H	-2.244836000	-2.665880000	1.928990000
H	-1.200920000	7.159951000	-0.373345000	H	-2.439209000	-1.466615000	3.969386000
H	-0.508793000	7.453025000	-2.750718000	H	-1.629748000	0.321398000	5.478522000
H	-1.688670000	1.696156000	2.138028000	H	0.569903000	1.428704000	5.061821000
H	-4.555464000	3.377842000	-0.636722000	H	1.985120000	0.692616000	3.151514000
H	-3.317108000	2.000322000	3.982684000	H	1.293131000	-1.213903000	1.751126000
H	-6.160040000	3.695049000	1.209695000				
H	-5.553936000	3.008272000	3.532064000				
H	-3.854816000	-0.745050000	1.321847000				
H	-4.931683000	-1.992690000	-2.678939000	Pd	-0.551718000	0.205770000	0.505847000
H	-6.253437000	-0.770013000	1.968063000	P	-2.488068000	-0.249429000	1.744032000
H	-7.317752000	-1.998359000	-2.031729000	C	-2.706127000	-2.101035000	1.812507000

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C	-2.949238000	-2.775845000	0.453554000	H	-1.691104000	1.076382000	-4.216548000
P	-1.643856000	-2.615957000	-0.868307000	H	-5.214209000	-1.414256000	-4.066035000
C	-0.181441000	-1.958246000	-0.095467000	H	-3.973613000	0.515562000	-5.048591000
C	-1.410453000	-4.290441000	-1.564070000	H	-3.262326000	1.318865000	-0.601692000
C	-1.307460000	-5.398255000	-0.702999000	H	-5.272256000	-0.519578000	2.764445000
C	-1.220431000	-4.467252000	-2.944402000	H	-5.454085000	2.062041000	-1.494049000
C	-1.047215000	-6.668416000	-1.219997000	H	-7.453044000	0.217373000	1.860192000
C	-0.960820000	-5.741293000	-3.455230000	H	-7.556988000	1.512792000	-0.268342000
C	-0.877684000	-6.841473000	-2.597578000	H	-0.999154000	-1.332810000	4.065354000
C	-2.359630000	-1.588412000	-2.193877000	H	-3.728243000	1.947019000	3.300919000
C	-1.659622000	-0.510753000	-2.757088000	H	-0.778992000	-0.596913000	6.404634000
C	-3.641023000	-1.911746000	-2.676409000	H	-3.473772000	2.687395000	5.647382000
C	-2.245585000	0.244435000	-3.776618000	H	-2.006107000	1.418701000	7.215904000
C	-4.219824000	-1.154374000	-3.696077000	H	1.764495000	-1.640321000	1.731723000
C	-3.523282000	-0.072895000	-4.245523000	H	3.319742000	-2.306662000	-2.230676000
C	-4.113268000	0.340877000	1.133304000	H	4.041040000	-1.653122000	2.641597000
C	-4.178416000	1.071513000	-0.063040000	H	5.632331000	-2.281632000	-1.320637000
C	-5.303221000	0.035926000	1.823323000	H	6.002880000	-0.431612000	2.769455000
C	-5.415557000	1.490287000	-0.564417000	H	7.139845000	-3.498910000	-0.052920000
C	-6.534496000	0.455462000	1.318432000	H	8.293201000	-0.444690000	3.701905000
C	-6.591401000	1.183164000	0.123072000	H	9.434596000	-3.489679000	0.866140000
C	-2.397310000	0.244294000	3.509888000	H	10.027629000	-1.968900000	2.754324000
C	-1.559139000	-0.455312000	4.398375000	C	1.936618000	2.855266000	-0.266907000
C	-3.076366000	1.385405000	3.972953000	C	-0.267819000	2.248955000	1.034076000
C	-1.425138000	-0.037314000	5.724062000	C	1.163000000	1.934134000	0.659551000
C	-2.933968000	1.803257000	5.299644000	C	2.091016000	4.211141000	0.059004000
C	-2.112364000	1.092812000	6.178609000	C	2.555065000	2.365614000	-1.428001000
C	1.015872000	-2.016861000	-0.955327000	C	2.841414000	5.057258000	-0.758330000
O	0.903244000	-2.076583000	-2.183010000	C	3.301052000	3.210781000	-2.246486000
C	2.377651000	-1.984630000	-0.325985000	C	3.453732000	4.568514000	-1.924158000
C	2.603694000	-1.790882000	1.049076000	C	-1.126276000	3.140181000	0.233531000
C	3.493507000	-2.164900000	-1.162438000	C	-1.064367000	3.206480000	-1.176763000
C	3.896975000	-1.781198000	1.566768000	C	-2.075491000	3.954644000	0.889239000
C	4.784523000	-2.158566000	-0.643529000	C	-1.916937000	4.046741000	-1.892730000
C	5.018715000	-1.967693000	0.733766000	C	-2.922549000	4.799648000	0.172830000
C	6.396224000	-1.965908000	1.288671000	C	-2.848884000	4.848576000	-1.223426000
C	6.745775000	-1.119055000	2.358239000	C	4.271761000	5.428279000	-2.855699000
C	7.389124000	-2.813406000	0.760192000	O	4.752906000	4.945920000	-3.860930000
C	8.040702000	-1.118333000	2.879241000	C	4.475215000	6.889856000	-2.509698000
C	8.682679000	-2.816197000	1.284703000	H	-0.423611000	2.365562000	2.112296000
C	9.014314000	-1.968133000	2.345590000	H	1.742157000	1.770269000	1.582321000
H	-1.815180000	-2.518384000	2.303749000	H	1.227934000	0.897822000	0.150784000
H	-3.560486000	-2.326477000	2.470934000	H	1.619490000	4.612200000	0.959667000
H	-3.883166000	-2.399931000	0.010278000	H	2.456132000	1.308515000	-1.693412000
H	-3.100501000	-3.853008000	0.615285000	H	2.943923000	6.107055000	-0.477274000
H	-0.057506000	-2.424104000	0.890374000	H	3.785018000	2.840449000	-3.152357000
H	-1.420145000	-5.283280000	0.378501000	H	-0.333156000	2.605127000	-1.718830000
H	-1.265870000	-3.611876000	-3.619400000	H	-2.135365000	3.928228000	1.980758000
H	-0.974415000	-7.524233000	-0.544988000	H	-1.844690000	4.087545000	-2.982435000
H	-0.817457000	-5.871823000	-4.530260000	H	-3.640021000	5.428511000	0.705641000
H	-0.675200000	-7.836160000	-3.001713000	H	-3.506067000	5.515623000	-1.786437000
H	-0.643683000	-0.291156000	-2.431379000	H	3.510668000	7.419860000	-2.449439000
H	-4.193733000	-2.764144000	-2.272575000	H	4.970683000	6.999581000	-1.531345000

H	5.096109000	7.353819000	-3.286130000	H	1.248536000	4.404541000	2.663178000
"10-trans"				H	2.023931000	4.834828000	-1.582323000
Pd	0.727683000	-0.396061000	-0.230988000	H	0.899598000	6.835832000	2.841607000
P	2.209321000	-0.756086000	1.552597000	H	1.664434000	7.277784000	-1.384108000
C	2.240293000	0.792645000	2.595147000	H	1.107786000	8.289630000	0.825630000
C	2.771063000	2.039411000	1.871260000	H	1.414139000	1.441625000	-2.317426000
P	1.855216000	2.635764000	0.362268000	H	4.659417000	3.280050000	-0.123737000
C	0.293100000	1.785760000	0.326447000	H	2.952427000	1.037864000	-4.229748000
C	1.695939000	4.449251000	0.527409000	H	6.171021000	2.898528000	-2.035667000
C	1.359707000	5.021961000	1.767875000	H	5.330842000	1.771991000	-4.097592000
C	1.793556000	5.269618000	-0.609054000	H	3.750653000	-0.993172000	-0.925740000
C	1.153157000	6.398398000	1.873255000	H	4.567634000	-1.172657000	3.322368000
C	1.584176000	6.646223000	-0.496467000	H	6.164186000	-1.303031000	-1.395302000
C	1.268733000	7.212250000	0.741578000	H	6.973813000	-1.469900000	2.843295000
C	2.939287000	2.338478000	-1.075245000	H	7.786533000	-1.542366000	0.486309000
C	2.465855000	1.716558000	-2.240573000	H	-0.113720000	-0.943608000	3.332110000
C	4.276800000	2.768852000	-1.011204000	H	3.270599000	-3.448074000	2.306019000
C	3.329439000	1.510999000	-3.320097000	H	-0.945312000	-2.699102000	4.851174000
C	5.134012000	2.560103000	-2.093106000	H	2.404656000	-5.211191000	3.808559000
C	4.661556000	1.927904000	-3.248046000	H	0.300729000	-4.847144000	5.096875000
C	3.988800000	-1.053770000	1.225494000	H	-2.054931000	1.614609000	1.724249000
C	4.453365000	-1.093791000	-0.097849000	H	-2.608570000	2.781125000	-2.387453000
C	4.908903000	-1.189373000	2.284047000	H	-4.476567000	1.487338000	2.028276000
C	5.816026000	-1.269026000	-0.360754000	H	-5.066928000	2.582099000	-2.105157000
C	6.267471000	-1.362913000	2.016526000	H	-6.347643000	0.252169000	1.559133000
C	6.722454000	-1.403576000	0.692752000	H	-6.908279000	3.561263000	-1.161624000
C	1.658771000	-2.055042000	2.727022000	H	-8.795034000	0.097755000	1.871497000
C	0.460649000	-1.867324000	3.442193000	H	-9.354624000	3.387938000	-0.862381000
C	2.346883000	-3.273365000	2.860337000	H	-10.318261000	1.658640000	0.657702000
C	-0.019270000	-2.862593000	4.294921000	C	-1.920724000	-2.388995000	-1.447303000
C	1.857208000	-4.270701000	3.710115000	C	0.584807000	-2.388087000	-0.962244000
C	0.678634000	-4.067260000	4.431722000	C	-0.557044000	-1.807326000	-1.757931000
C	-0.676884000	2.343544000	-0.631931000	C	-2.767819000	-1.804769000	-0.498404000
O	-0.290813000	2.907439000	-1.659734000	C	-2.339939000	-3.557507000	-2.106570000
C	-2.148663000	2.193737000	-0.371956000	C	-4.012894000	-2.371259000	-0.213581000
C	-2.699284000	1.820755000	0.867204000	C	-3.578022000	-4.123700000	-1.818995000
C	-3.032554000	2.482601000	-1.427030000	C	-4.432968000	-3.537910000	-0.869136000
C	-4.079418000	1.738751000	1.042637000	C	1.770068000	-2.937919000	-1.648693000
C	-4.409545000	2.384411000	-1.256100000	C	2.253732000	-2.427301000	-2.873487000
C	-4.968511000	2.011965000	-0.016080000	C	2.454933000	-4.031320000	-1.076685000
C	-6.439213000	1.915472000	0.170116000	C	3.370355000	-2.986722000	-3.494713000
C	-6.999969000	0.952098000	1.031625000	C	3.569875000	-4.592442000	-1.699414000
C	-7.314072000	2.785621000	-0.508533000	C	4.034690000	-4.072417000	-2.911748000
C	-8.382167000	0.858342000	1.204088000	C	-5.765085000	-4.197123000	-0.614701000
C	-8.696035000	2.695153000	-0.332885000	O	-6.063466000	-5.214586000	-1.206075000
C	-9.236480000	1.730155000	0.522123000	C	-6.712724000	-3.564009000	0.386073000
H	1.220454000	0.958790000	2.973076000	H	0.261745000	-3.000494000	-0.111913000
H	2.872030000	0.605980000	3.478441000	H	-0.351863000	-1.852052000	-2.837366000
H	3.812758000	1.877676000	1.556495000	H	-0.651207000	-0.666912000	-1.581303000
H	2.794372000	2.879822000	2.579978000	H	-2.465511000	-0.883681000	0.006439000
H	-0.072551000	1.670343000	1.352298000	H	-1.690862000	-4.023932000	-2.852985000
				H	-4.657849000	-1.884418000	0.519643000
				H	-3.917648000	-5.029709000	-2.324830000

H	1.751750000	-1.581860000	-3.350719000
H	2.090593000	-4.454440000	-0.136821000
H	3.720757000	-2.579393000	-4.446452000
H	4.073540000	-5.447729000	-1.242328000
H	4.902231000	-4.516340000	-3.405602000
H	-6.253117000	-3.513742000	1.386778000
H	-6.971548000	-2.534184000	0.090527000
H	-7.626499000	-4.169114000	0.437144000

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Pd	-0.518600000	0.228191000	0.441961000
P	-2.486890000	-0.659083000	1.658376000
C	-2.389185000	-2.521304000	1.620796000
C	-2.483148000	-3.100424000	0.202139000
P	-1.143114000	-2.671318000	-1.021690000
C	0.156846000	-1.778845000	-0.153524000
C	-0.570143000	-4.269578000	-1.697555000
C	-0.320269000	-5.340456000	-0.819937000
C	-0.294096000	-4.416570000	-3.066465000
C	0.176684000	-6.549163000	-1.310772000
C	0.197773000	-5.630536000	-3.551335000
C	0.431435000	-6.696486000	-2.677982000
C	-1.925906000	-1.741058000	-2.377255000
C	-1.392296000	-0.529492000	-2.841753000
C	-3.081151000	-2.271322000	-2.980175000
C	-2.019006000	0.149328000	-3.890158000
C	-3.700791000	-1.587876000	-4.027906000
C	-3.170889000	-0.375749000	-4.482688000
C	-4.208736000	-0.353492000	1.099956000
C	-4.425942000	0.458214000	-0.024547000
C	-5.312284000	-0.954213000	1.737559000
C	-5.723205000	0.666091000	-0.505463000
C	-6.604802000	-0.743541000	1.255282000
C	-6.811365000	0.066503000	0.131629000
C	-2.443623000	-0.269876000	3.455786000
C	-1.371374000	-0.748393000	4.233091000
C	-3.390398000	0.577432000	4.056450000
C	-1.267260000	-0.412215000	5.584305000
C	-3.277872000	0.917994000	5.408721000
C	-2.221424000	0.422014000	6.176258000
C	1.399457000	-1.735030000	-0.978201000
O	1.317694000	-1.846320000	-2.200427000
C	2.734878000	-1.575404000	-0.318615000
C	2.913186000	-1.384553000	1.063225000
C	3.878491000	-1.629791000	-1.134880000
C	4.188808000	-1.260233000	1.607677000
C	5.152406000	-1.503183000	-0.589660000
C	5.339690000	-1.316674000	0.795187000
C	6.699337000	-1.185206000	1.377944000
C	6.940014000	-0.332093000	2.472358000
C	7.784786000	-1.910857000	0.849874000
C	8.218811000	-0.208145000	3.017836000

C	9.062548000	-1.790389000	1.398555000
C	9.285294000	-0.937868000	2.484057000
H	-1.454154000	-2.822937000	2.116019000
H	-3.209577000	-2.938359000	2.225682000
H	-3.431367000	-2.794318000	-0.264615000
H	-2.509664000	-4.198237000	0.257834000
H	0.299307000	-2.245520000	0.830890000
H	-0.503139000	-5.243587000	0.253859000
H	-0.452291000	-3.583169000	-3.751613000
H	0.365567000	-7.376917000	-0.623440000
H	0.406236000	-5.739644000	-4.618042000
H	0.817424000	-7.643732000	-3.062011000
H	-0.477921000	-0.132309000	-2.401992000
H	-3.500462000	-3.225099000	-2.648608000
H	-1.593103000	1.087138000	-4.254201000
H	-4.595778000	-2.006736000	-4.493507000
H	-3.652757000	0.154949000	-5.307416000
H	-3.580818000	0.935694000	-0.523341000
H	-5.168735000	-1.581675000	2.621337000
H	-5.878345000	1.302446000	-1.379414000
H	-7.454827000	-1.211317000	1.757943000
H	-7.824661000	0.229946000	-0.243488000
H	-0.603832000	-1.387801000	3.788212000
H	-4.225359000	0.970101000	3.473158000
H	-0.435359000	-0.800977000	6.176512000
H	-4.025601000	1.572299000	5.863564000
H	-2.138831000	0.686030000	7.233129000
H	2.050053000	-1.323034000	1.728734000
H	3.741240000	-1.769133000	-2.208642000
H	4.298646000	-1.139047000	2.687262000
H	6.020391000	-1.526185000	-1.251760000
H	6.122866000	0.264669000	2.884187000
H	7.622549000	-2.598338000	0.016694000
H	8.385268000	0.468565000	3.859649000
H	9.888217000	-2.370609000	0.979322000
H	10.286225000	-0.841774000	2.911612000
C	1.210309000	3.197403000	-0.157318000
C	-0.841190000	2.417469000	1.213265000
C	0.508161000	2.359995000	0.865867000
C	0.969144000	4.583332000	-0.175705000
C	2.212238000	2.686197000	-1.003089000
C	1.692832000	5.425287000	-1.021964000
C	2.928356000	3.524874000	-1.850727000
C	2.678056000	4.907175000	-1.875663000
C	-1.924711000	3.118437000	0.489590000
C	-1.953537000	3.257281000	-0.913330000
C	-2.983563000	3.670869000	1.235972000
C	-2.995533000	3.941562000	-1.539002000
C	-4.022554000	4.362072000	0.608947000
C	-4.031845000	4.501702000	-0.781598000
C	3.490290000	5.757597000	-2.821236000
O	4.306792000	5.237365000	-3.554061000
C	3.265065000	7.256335000	-2.830890000

H	-1.076646000	2.157088000	2.249942000
H	1.176281000	1.971428000	1.644121000
H	0.837365000	0.613774000	-0.212779000
H	0.216019000	5.011938000	0.488000000
H	2.429599000	1.614964000	-1.001281000
H	1.479829000	6.495701000	-1.005037000
H	3.700075000	3.130122000	-2.514383000
H	-1.153373000	2.826079000	-1.517188000
H	-2.983021000	3.566389000	2.324404000
H	-2.998441000	4.043001000	-2.627146000
H	-4.827336000	4.793430000	1.209074000
H	-4.842172000	5.043874000	-1.274856000
H	2.222958000	7.498487000	-3.096004000
H	3.459151000	7.691428000	-1.837018000
H	3.941258000	7.710898000	-3.565563000

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Pd	0.707801000	-0.417011000	-0.288940000
P	2.182676000	-0.876584000	1.478632000
C	2.132116000	0.569382000	2.656025000
C	2.638726000	1.897633000	2.073986000
P	1.775922000	2.592932000	0.575732000
C	0.236310000	1.716460000	0.389334000
C	1.548277000	4.378678000	0.892569000
C	1.084487000	4.813547000	2.147681000
C	1.718166000	5.312041000	-0.143346000
C	0.824398000	6.166596000	2.370400000
C	1.454806000	6.664834000	0.086185000
C	1.013106000	7.094086000	1.340417000
C	2.942109000	2.452959000	-0.819542000
C	2.561262000	1.905006000	-2.053463000
C	4.251159000	2.939355000	-0.649715000
C	3.487458000	1.829083000	-3.097214000
C	5.170684000	2.862686000	-1.697124000
C	4.789934000	2.304588000	-2.922036000
C	3.975034000	-1.084268000	1.153227000
C	4.458362000	-0.975298000	-0.159344000
C	4.882712000	-1.308293000	2.207357000
C	5.828893000	-1.088514000	-0.416338000
C	6.248997000	-1.418457000	1.945957000
C	6.723411000	-1.308763000	0.632814000
C	1.687516000	-2.301033000	2.526689000
C	0.555068000	-2.206775000	3.357153000
C	2.366736000	-3.529333000	2.441917000
C	0.129455000	-3.307791000	4.103030000
C	1.932215000	-4.630842000	3.185382000
C	0.816295000	-4.523058000	4.019092000
C	-0.677777000	2.350451000	-0.580360000
O	-0.225946000	2.995688000	-1.530731000
C	-2.162417000	2.195475000	-0.425440000
C	-2.791091000	1.707077000	0.733632000
C	-2.978073000	2.615366000	-1.491974000

C	-4.180112000	1.643198000	0.822458000
C	-4.364106000	2.537017000	-1.408351000
C	-5.000837000	2.052007000	-0.247351000
C	-6.481249000	1.983977000	-0.150170000
C	-7.114880000	0.946385000	0.560868000
C	-7.292092000	2.958138000	-0.764151000
C	-8.506129000	0.883806000	0.653758000
C	-8.683374000	2.897940000	-0.668132000
C	-9.296594000	1.860278000	0.040238000
H	1.095088000	0.668139000	3.008996000
H	2.740372000	0.320984000	3.540737000
H	3.702237000	1.811244000	1.805969000
H	2.583450000	2.670387000	2.854503000
H	-0.188084000	1.534792000	1.383630000
H	0.912503000	4.103450000	2.961133000
H	2.047034000	4.984479000	-1.130285000
H	0.471137000	6.496902000	3.349926000
H	1.591574000	7.385223000	-0.723493000
H	0.809808000	8.153131000	1.515928000
H	1.531446000	1.585542000	-2.208978000
H	4.561688000	3.394490000	0.294543000
H	3.182550000	1.410332000	-4.058830000
H	6.184195000	3.245434000	-1.557463000
H	5.507527000	2.251398000	-3.744388000
H	3.764371000	-0.805841000	-0.983569000
H	4.525021000	-1.411090000	3.235197000
H	6.192340000	-1.006945000	-1.442870000
H	6.946370000	-1.594226000	2.768568000
H	7.793614000	-1.398774000	0.430973000
H	-0.009672000	-1.273874000	3.429234000
H	3.246296000	-3.628102000	1.802950000
H	-0.745441000	-3.216116000	4.751060000
H	2.473857000	-5.577117000	3.113979000
H	0.480745000	-5.384071000	4.601740000
H	-2.201035000	1.394917000	1.597941000
H	-2.493439000	3.003878000	-2.389404000
H	-4.639576000	1.299409000	1.751419000
H	-4.968197000	2.842466000	-2.265092000
H	-6.511561000	0.162557000	1.024918000
H	-6.828594000	3.789110000	-1.300561000
H	-8.976997000	0.064126000	1.202253000
H	-9.292151000	3.670648000	-1.143969000
H	-10.385691000	1.812482000	0.113591000
C	-1.917748000	-2.440283000	-1.338055000
C	0.623389000	-2.349817000	-1.167461000
C	-0.629035000	-1.795441000	-1.800138000
C	-2.548217000	-2.035512000	-0.155085000
C	-2.480060000	-3.490906000	-2.082044000
C	-3.715229000	-2.665932000	0.281396000
C	-3.641515000	-4.122011000	-1.645574000
C	-4.275036000	-3.719360000	-0.457543000
C	1.789469000	-2.687243000	-2.005415000
C	2.112574000	-1.978312000	-3.183605000

C	2.622194000	-3.765618000	-1.637180000
C	3.220268000	-2.332597000	-3.954003000
C	3.726773000	-4.122633000	-2.410133000
C	4.033374000	-3.406101000	-3.571959000
C	-5.531817000	-4.443260000	-0.045091000
O	-5.954772000	-5.361338000	-0.717195000
C	-6.249283000	-3.999421000	1.215893000
H	0.434090000	-3.082039000	-0.374227000
H	-0.556949000	-1.801017000	-2.897612000
H	-0.736247000	-0.661423000	-1.582691000
H	-2.133801000	-1.200816000	0.416298000
H	-2.002970000	-3.815872000	-3.010768000
H	-4.189991000	-2.322784000	1.202271000
H	-4.088829000	-4.940072000	-2.213640000
H	1.488346000	-1.141607000	-3.507708000
H	2.381969000	-4.339661000	-0.738359000
H	3.445687000	-1.775223000	-4.866693000
H	4.347295000	-4.970762000	-2.110645000
H	4.893002000	-3.689898000	-4.183616000
H	-5.593020000	-4.083444000	2.097311000
H	-6.564649000	-2.946065000	1.138650000
H	-7.133162000	-4.633241000	1.359615000

“12-cis”

Pd	-0.722081000	0.568964000	-0.032871000
P	-2.522907000	0.935045000	1.662906000
C	-2.709817000	-0.643460000	2.632232000
C	-3.156068000	-1.830333000	1.766623000
P	-2.052829000	-2.397682000	0.371019000
C	-0.467871000	-1.539310000	0.479172000
C	-1.887943000	-4.204265000	0.595646000
C	-1.623673000	-4.719983000	1.877483000
C	-1.937030000	-5.074847000	-0.505108000
C	-1.435396000	-6.091626000	2.057552000
C	-1.754664000	-6.446514000	-0.316566000
C	-1.506478000	-6.956453000	0.961039000
C	-2.971776000	-2.103391000	-1.173920000
C	-2.416063000	-1.373705000	-2.235017000
C	-4.271744000	-2.628054000	-1.293106000
C	-3.163250000	-1.151710000	-3.394873000
C	-5.009594000	-2.410185000	-2.458085000
C	-4.456974000	-1.668967000	-3.508335000
C	-4.251013000	1.327534000	1.177392000
C	-4.593352000	1.309447000	-0.185107000
C	-5.248816000	1.603292000	2.131987000
C	-5.909291000	1.562878000	-0.587655000
C	-6.560059000	1.857006000	1.726535000
C	-6.891745000	1.837652000	0.366149000
C	-2.065650000	2.189387000	2.927160000
C	-1.141437000	1.883785000	3.943939000
C	-2.533576000	3.511610000	2.814697000
C	-0.715735000	2.870388000	4.837497000

C	-2.101192000	4.496285000	3.707595000
C	-1.194198000	4.178832000	4.722379000
C	0.528039000	-2.229568000	-0.400318000
O	0.114501000	-2.900970000	-1.344645000
C	1.992449000	-2.128436000	-0.120893000
C	2.546800000	-1.326022000	0.891700000
C	2.865359000	-2.880332000	-0.927556000
C	3.924581000	-1.272199000	1.084333000
C	4.241506000	-2.827233000	-0.732243000
C	4.805767000	-2.015559000	0.273129000
C	6.276414000	-1.932292000	0.460707000
C	6.890615000	-0.710496000	0.797771000
C	7.093690000	-3.066801000	0.291068000
C	8.275348000	-0.626065000	0.954173000
C	8.477092000	-2.982908000	0.457890000
C	9.073758000	-1.761674000	0.787981000
H	-1.746274000	-0.854817000	3.119574000
H	-3.446102000	-0.497226000	3.438789000
H	-4.132344000	-1.614456000	1.306771000
H	-3.310250000	-2.707596000	2.411223000
H	-0.167279000	-1.483901000	1.535292000
H	-1.553841000	-4.060538000	2.746878000
H	-2.104696000	-4.681860000	-1.508128000
H	-1.232210000	-6.484561000	3.056321000
H	-1.799203000	-7.118869000	-1.176328000
H	-1.362695000	-8.030189000	1.102985000
H	-1.399552000	-0.987511000	-2.160289000
H	-4.714096000	-3.218971000	-0.486564000
H	-2.723004000	-0.578706000	-4.213900000
H	-6.016813000	-2.823789000	-2.546251000
H	-5.035179000	-1.501645000	-4.420385000
H	-3.831994000	1.087305000	-0.936298000
H	-5.001893000	1.632591000	3.196515000
H	-6.163423000	1.544093000	-1.649964000
H	-7.326919000	2.073368000	2.474239000
H	-7.918925000	2.038881000	0.052378000
H	-0.742639000	0.872531000	4.053183000
H	-3.250952000	3.777260000	2.034886000
H	-0.006470000	2.613173000	5.627858000
H	-2.480438000	5.516402000	3.610452000
H	-0.860704000	4.948719000	5.421973000
H	1.903406000	-0.717478000	1.529619000
H	2.436260000	-3.498266000	-1.718167000
H	4.330687000	-0.649922000	1.884058000
H	4.897910000	-3.401127000	-1.389735000
H	6.295170000	0.198228000	0.905895000
H	6.639304000	-4.031142000	0.051409000
H	8.725490000	0.339887000	1.195218000
H	9.092406000	-3.877552000	0.333592000
H	10.157459000	-1.696207000	0.912984000
C	1.528171000	2.917256000	-0.384664000
C	-0.955939000	2.679316000	-1.187910000
C	0.057755000	2.815200000	-0.254172000

C	2.182829000	3.394921000	-1.534469000	C	5.348422000	0.402537000	0.789720000
C	2.312527000	2.611292000	0.747424000	C	5.493843000	-0.042637000	3.165903000
C	3.572888000	3.515882000	-1.563542000	C	6.103860000	0.331379000	1.961743000
C	3.696720000	2.710261000	0.709925000	C	1.355732000	-2.105502000	3.072006000
C	4.351288000	3.151658000	-0.452786000	C	0.248759000	-2.265420000	3.924033000
C	-0.949144000	2.479285000	-2.654090000	C	2.274029000	-3.165350000	2.949526000
C	0.033425000	1.758903000	-3.365202000	C	0.075792000	-3.448177000	4.649228000
C	-2.023337000	3.030073000	-3.382609000	C	2.094940000	-4.348162000	3.671430000
C	-0.046885000	1.621868000	-4.750295000	C	0.996853000	-4.492139000	4.525298000
C	-2.098333000	2.900879000	-4.771183000	C	-1.718901000	1.803259000	-0.590924000
C	-1.108521000	2.196516000	-5.461386000	O	-1.374261000	2.743198000	-1.304500000
C	5.856733000	3.200241000	-0.442340000	C	-3.082508000	1.203825000	-0.728088000
O	6.471139000	2.713175000	0.488550000	C	-3.523311000	0.078747000	-0.010133000
C	6.577507000	3.850690000	-1.603979000	C	-3.982813000	1.826074000	-1.611242000
H	-1.946914000	2.951060000	-0.808522000	C	-4.824280000	-0.395839000	-0.159497000
H	-0.288669000	3.096904000	0.746559000	C	-5.281217000	1.350168000	-1.759517000
H	0.494212000	0.215151000	-0.930639000	C	-5.735723000	0.229878000	-1.033630000
H	1.604877000	3.693869000	-2.409039000	C	-7.125211000	-0.273009000	-1.184624000
H	1.818441000	2.282196000	1.665562000	C	-7.411448000	-1.649923000	-1.108360000
H	4.047518000	3.894246000	-2.470783000	C	-8.195293000	0.615288000	-1.406858000
H	4.305002000	2.454811000	1.579402000	C	-8.717254000	-2.121419000	-1.252445000
H	0.856172000	1.286878000	-2.827171000	C	-9.501898000	0.144396000	-1.546025000
H	-2.804140000	3.580945000	-2.850771000	C	-9.768593000	-1.225953000	-1.470855000
H	0.724036000	1.057746000	-5.280913000	H	-0.566711000	-0.253369000	-1.415249000
H	-2.933132000	3.350718000	-5.314032000	H	-0.160433000	0.608725000	3.288338000
H	-1.163660000	2.090137000	-6.547474000	H	1.403622000	0.696510000	4.106722000
H	6.392060000	3.292849000	-2.536714000	H	2.257195000	2.298370000	2.359389000
H	6.227524000	4.882910000	-1.764648000	H	0.901550000	2.926213000	3.287746000
H	7.654957000	3.853333000	-1.397559000	H	-1.292865000	0.937798000	1.362013000

“12-trans”

Pd	0.296543000	-0.499889000	-0.141078000	H	-2.606721000	5.488981000	3.774295000
P	1.553509000	-0.602676000	2.029483000	H	-1.471708000	7.174336000	-0.034995000
C	0.915549000	0.769128000	3.121655000	H	-2.703490000	7.357849000	2.125095000
C	1.180510000	2.165772000	2.544278000	H	0.971172000	1.669874000	-1.762641000
P	0.323574000	2.644065000	0.959272000	H	2.514813000	4.553649000	1.073752000
C	-0.779018000	1.303799000	0.461883000	H	2.800329000	2.259011000	-3.338234000
C	-0.594920000	4.177457000	1.341434000	H	4.328628000	5.132464000	-0.499656000
C	-1.305055000	4.277440000	2.551955000	H	4.481193000	3.993913000	-2.714043000
C	-0.669662000	5.222599000	0.405979000	H	3.399600000	0.152460000	-0.104602000
C	-2.060433000	5.417979000	2.831016000	H	3.672146000	-0.646786000	4.141707000
C	-1.422219000	6.363046000	0.694793000	H	5.820325000	0.686562000	-0.153503000
C	-2.115227000	6.463959000	1.904548000	H	6.083980000	-0.102858000	4.083558000
C	1.629314000	3.054340000	-0.238057000	H	7.171532000	0.562969000	1.939788000
C	1.712391000	2.419269000	-1.484852000	H	-0.492908000	-1.471529000	4.033834000
C	2.575148000	4.035068000	0.113063000	H	3.147398000	-3.063631000	2.301050000
C	2.741181000	2.756665000	-2.367994000	H	-0.783762000	-3.551090000	5.315950000
C	3.598489000	4.368380000	-0.775804000	H	2.821738000	-5.157844000	3.571152000
C	3.682306000	3.728777000	-2.017316000	H	0.861869000	-5.414441000	5.095123000
C	3.362121000	-0.275154000	2.019222000	H	-2.848852000	-0.447336000	0.667622000
C	3.982185000	0.100350000	0.816846000	H	-3.636467000	2.692270000	-2.177607000
C	4.131896000	-0.344440000	3.197078000	H	-5.145405000	-1.257991000	0.427914000
				H	-5.952053000	1.841880000	-2.466985000

H	-6.597404000	-2.363281000	-0.960415000
H	-8.007318000	1.690605000	-1.444375000
H	-8.914752000	-3.195089000	-1.201079000
H	-10.317933000	0.853027000	-1.707665000
H	-10.791177000	-1.594465000	-1.582121000
C	1.309583000	-2.479215000	-0.990832000
C	-0.030164000	-2.562171000	-1.333711000
C	2.388253000	-2.076684000	-1.913581000
C	3.717682000	-2.423406000	-1.594902000
C	2.158156000	-1.396082000	-3.127596000
C	4.769257000	-2.109964000	-2.449339000
C	3.210866000	-1.089719000	-3.986774000
C	4.533964000	-1.437322000	-3.659486000
C	-1.091797000	-3.290489000	-0.617485000
C	-2.345913000	-3.423222000	-1.246401000
C	-0.904987000	-3.908191000	0.636255000
C	-3.374931000	-4.154425000	-0.652370000
C	-1.936296000	-4.632335000	1.231940000
C	-3.174708000	-4.761064000	0.591138000
C	5.717995000	-1.123793000	-4.538046000
O	6.841882000	-1.377413000	-4.153341000
C	5.474045000	-0.495319000	-5.895775000
H	1.647804000	-3.000456000	-0.091643000
H	-0.308144000	-2.271415000	-2.348787000
H	3.922233000	-2.959415000	-0.664408000
H	1.145624000	-1.099502000	-3.408035000
H	5.797695000	-2.382293000	-2.204224000
H	2.991465000	-0.572979000	-4.923202000
H	-2.511112000	-2.948976000	-2.217335000
H	0.052356000	-3.831409000	1.153386000
H	-4.334141000	-4.255277000	-1.165809000
H	-1.768982000	-5.108103000	2.200912000
H	-3.976782000	-5.337994000	1.057728000
H	4.824685000	-1.134178000	-6.516130000
H	4.972731000	0.481447000	-5.797575000
H	6.438479000	-0.356832000	-6.400063000

