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Supporting Information-2

Theoretical and experimental studies on visible light driven metal free regioselective functionalization of 1, 4-quinones with diazo esters

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Coordinates

For BQ
(for highlighted pathways)

FOR A(X=H)

Benzoquinone(BQ)

C	-3.250300	1.089000	0.000000
C	-3.285700	-0.252700	0.000000
C	-1.950200	1.799400	0.000000
C	-0.689400	1.021400	0.000000
C	-0.724800	-0.320300	0.000000
C	-2.024900	-1.030800	0.000000
O	-1.918000	3.019400	0.000000
O	-2.057100	-2.250800	0.000000
H	0.266500	1.536700	0.000000
H	0.202500	-0.885400	0.000000
H	-4.241600	-0.768100	0.000000
H	-4.177600	1.654000	0.000000

Hcarbene

C	-1.824100	-0.802200	0.000000
H	-2.636300	-0.054500	-0.000100
C	-0.568700	0.052900	0.000000
O	-0.537100	1.270600	0.000000
O	0.523600	-0.718300	0.000000
C	1.797300	-0.036600	0.000000
H	2.547600	-0.821800	0.000000
H	1.884900	0.586800	0.890700
H	1.884900	0.586800	-0.890800

EPInt

C	-1.454100	1.269100	0.000000
C	-2.813400	1.324800	0.000000
C	-0.795000	0.010600	-0.000200
C	-1.526900	-1.206000	-0.000200
C	-2.887200	-1.158200	-0.000100
C	-3.621900	0.110600	0.000100
O	-4.865800	0.138400	0.000200
H	-0.845200	2.165700	0.000000
H	-3.335300	2.274000	0.000100

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 H   -1.017800   -2.161600   -0.000300
 H   -3.474500   -2.068700   -0.000200
 C    2.833700   -0.529600    0.000100
 O    3.700600   -1.389300    0.000300
 O    3.066200    0.791000    0.000000
 C    4.453100    1.196600   -0.000100
 H    4.955800    0.821500   -0.891600
 H    4.955600    0.822700    0.892100
 H    4.432800    2.283100   -0.000800
 O    0.540300    0.076600   -0.000100
 C    1.423300   -0.876700   -0.000100
 H    1.127500   -1.916000   -0.000100

EPTS
 C    1.821300   -1.470300   -0.263500
 C    3.043100   -0.916900   -0.040400
 C    0.688100   -0.620700   -0.360300
 C    0.812900    0.797700   -0.277900
 C    2.036000    1.359200   -0.068000
 C    3.226500    0.538500    0.090800
 O    4.354100    1.019700    0.294100
 H    1.682800   -2.540700   -0.358600
 H    3.931400   -1.532200    0.043000
 H   -0.068500    1.407300   -0.436800
 H    2.160900    2.434600   -0.042800
 C   -2.438300   -0.120900    0.562500
 O   -3.052900    0.106500    1.590800
 O   -2.859600    0.186100   -0.671400
 C   -4.162300    0.805400   -0.770200
 H   -4.169400    1.750900   -0.227500
 H   -4.925500    0.140900   -0.365100
 H   -4.321100    0.970700   -1.832100
 O   -0.553900   -1.191300   -0.580700
 C   -1.141000   -0.787600    0.568500
 H   -0.711200   -1.106200    1.507800

EP prod
 C    0.663200   -0.838900   -0.823400
 C    1.867700   -0.445600   -1.259200
 C    0.216200   -0.539000    0.552100
 C    1.196700    0.091400    1.459300
 C    2.398300    0.486300    1.018300
 C    2.812900    0.276800   -0.384100
 O   -0.660000   -1.524400    1.158900
 C   -1.246500   -0.290400    0.831800
 C   -2.271100   -0.298200   -0.282900
 O   -2.615800   -1.307800   -0.845200
 O   -2.808000    0.880500   -0.627200
 C   -2.371400    2.126800   -0.030700
 H   -2.844600    2.903700   -0.625000
 H   -1.288000    2.232600   -0.089800
 H   -2.714600    2.197900    1.002200
 O    3.900900    0.669700   -0.797500
 H   -0.022200   -1.385100   -1.460600
 H    0.896000    0.227600    2.492600
 H    2.200100   -0.650400   -2.270200
 H    3.116800    0.964900    1.673400
 H   -1.476000    0.349700    1.679400
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For B(CO_2Me)

Benzoquinone(BQ)

C	-3.250300	1.089000	0.000000
C	-3.285700	-0.252700	0.000000
C	-1.950200	1.799400	0.000000
C	-0.689400	1.021400	0.000000
C	-0.724800	-0.320300	0.000000
C	-2.024900	-1.030800	0.000000
O	-1.918000	3.019400	0.000000
O	-2.057100	-2.250800	0.000000
H	0.266500	1.536700	0.000000
H	0.202500	-0.885400	0.000000
H	-4.241600	-0.768100	0.000000
H	-4.177600	1.654000	0.000000

CO2Me carbene

C	-1.255300	-0.333900	0.211100
C	0.000400	-0.374700	0.906100
C	1.255100	-0.337300	0.207200
O	-1.640100	-1.391000	-0.264800
O	1.640600	-1.390000	-0.276500
O	-1.898000	0.821600	0.230500
O	1.897700	0.818900	0.234200
C	-3.227700	0.846600	-0.364800
C	3.227300	0.848600	-0.360700
H	3.581000	1.862300	-0.198600
H	3.163100	0.627700	-1.425000
H	3.873100	0.128500	0.139600
H	-3.582300	1.860900	-0.208600
H	-3.872900	0.128800	0.139400
H	-3.162800	0.619800	-1.427800

EPINT

C	-2.117700	-1.456900	0.438500
C	-3.461600	-1.298100	0.393500
C	-1.247200	-0.391100	0.038400
C	-1.775400	0.829300	-0.483100
C	-3.120400	0.983300	-0.560500
C	-4.056200	-0.054400	-0.101800
O	-5.280500	0.114000	-0.155400
H	-1.659500	-2.371900	0.794000
H	-4.136100	-2.083300	0.712000
H	-1.116400	1.604400	-0.840400
H	-3.554300	1.882900	-0.980200
C	2.354600	-0.934200	-0.043500
O	3.507800	-0.559200	0.039400
O	2.000000	-2.224900	-0.194800
C	3.083200	-3.178600	-0.220200
H	3.646800	-3.139300	0.712200
H	3.747800	-2.974200	-1.059800
H	2.606800	-4.148400	-0.338000
O	0.031600	-0.699400	0.139800
C	1.180400	-0.047200	0.005100
C	1.266700	1.407500	0.228000
O	2.347200	1.954400	-0.328600
O	0.444700	2.026100	0.881400
C	2.579200	3.353800	-0.044400
H	3.491700	3.603600	-0.578600
H	1.744500	3.955600	-0.403500
H	2.708800	3.502500	1.027600

EPTS

C	2.010600	0.063700	1.387800
C	3.211400	0.077000	0.762600
C	0.901500	-0.569700	0.750000
C	1.054400	-1.257900	-0.501100
C	2.256200	-1.259000	-1.129700
C	3.407700	-0.566800	-0.554900
O	4.510800	-0.537200	-1.109300
H	1.849300	0.536800	2.347100
H	4.077100	0.554500	1.206200
H	0.206100	-1.801200	-0.896600
H	2.407400	-1.794500	-2.058500
C	-2.225800	-0.585700	-0.069900
O	-3.147400	-0.042300	-0.643000
O	-2.178200	-1.904200	0.197900
C	-3.331800	-2.676300	-0.203300
H	-3.475600	-2.606400	-1.281700
H	-4.222700	-2.315600	0.311000
H	-3.107700	-3.698600	0.089100
O	-0.299200	-0.588000	1.406500
C	-1.023100	0.093400	0.450500
C	-0.758200	1.546700	0.324200
O	-1.311300	2.067600	-0.774000
O	-0.112500	2.185300	1.133900
C	-1.169300	3.495500	-0.949100
H	-1.686000	3.720200	-1.878300
H	-1.631200	4.025000	-0.115800
H	-0.115300	3.764200	-1.019500

EP prod

C	-1.596900	-1.294800	-0.324600
C	-2.903200	-1.170700	-0.060100
C	-0.721700	-0.108700	-0.463300
C	-1.385500	1.214200	-0.442800
C	-2.691200	1.331500	-0.170400
C	-3.543200	0.152100	0.082100
O	0.372200	-0.254600	-1.415500
C	0.731900	-0.227800	-0.052900
O	-4.731500	0.265500	0.367200
C	1.198400	-1.536700	0.602600
C	1.511000	0.969800	0.480900
O	1.990700	0.970100	1.589300
O	0.694300	-1.941300	1.618500
O	2.187400	-2.216300	0.018200
O	1.606200	1.952700	-0.405400
C	2.884700	-1.734000	-1.161000
C	2.339400	3.134800	0.015300
H	2.305200	3.806100	-0.837600
H	3.366400	2.864600	0.256800
H	1.855200	3.581700	0.882600
H	3.722500	-2.414700	-1.283700
H	3.261300	-0.722700	-1.005900
H	2.231500	-1.774300	-2.029900
H	-1.143400	-2.270400	-0.450400
H	-3.543800	-2.037900	0.048900
H	-3.177700	2.299400	-0.139400
H	-0.773200	2.080600	-0.654900

For C(Ph)

Benzoquinone(BQ)

C	-3.250300	1.089000	0.000000
C	-3.285700	-0.252700	0.000000
C	-1.950200	1.799400	0.000000
C	-0.689400	1.021400	0.000000
C	-0.724800	-0.320300	0.000000
C	-2.024900	-1.030800	0.000000
O	-1.918000	3.019400	0.000000
O	-2.057100	-2.250800	0.000000
H	0.266500	1.536700	0.000000
H	0.202500	-0.885400	0.000000
H	-4.241600	-0.768100	0.000000
H	-4.177600	1.654000	0.000000

Ph carbene

C	0.538000	-1.109100	0.003900
C	1.745600	-0.387500	0.282800
C	-0.722700	-0.471000	-0.000400
C	-0.905000	0.931200	0.187500
C	-1.876600	-1.274100	-0.221400
C	-2.169000	1.489400	0.153200
C	-3.283000	0.668900	-0.071600
C	-3.140400	-0.709400	-0.260000
O	2.169300	-0.289900	1.431400
O	2.410700	0.042000	-0.807300
C	3.737000	0.577700	-0.589900
H	4.107700	0.831200	-1.580000
H	4.377300	-0.171800	-0.124200
H	3.692800	1.467400	0.038200
H	-1.734300	-2.338800	-0.360000
H	-4.272400	1.111700	-0.099100
H	-4.014000	-1.326200	-0.431400
H	-0.038800	1.558700	0.361900
H	-2.303200	2.554700	0.296800

CHTS1/CPTS1

C	-2.404800	-1.420200	-1.107300
C	-3.184500	-0.630200	-0.351600
C	-1.171100	-2.018200	-0.549400
C	-0.690100	-1.432400	0.733100
C	-1.525500	-0.695100	1.528700
C	-2.830100	-0.261800	1.044200
O	-0.622200	-2.979500	-1.070700
O	-3.626400	0.367000	1.746400
H	-2.684900	-1.719400	-2.111300
H	-4.127200	-0.240400	-0.721000
H	0.197600	-1.886100	1.152500
H	-1.235500	-0.391200	2.527200
C	0.486700	0.088500	-0.417700
C	-0.165300	1.332400	-0.765100
C	1.859900	0.043600	-0.058800
O	0.057500	1.809300	-1.872900
O	-1.041700	1.839900	0.111100
C	-1.790100	3.001200	-0.329100
H	-2.467700	3.226500	0.490000
H	-2.346100	2.771000	-1.237400
H	-1.114600	3.837300	-0.509000
C	2.539800	-1.204900	-0.087500
C	2.602800	1.209300	0.279000
C	3.890400	-1.280800	0.203300
C	4.594200	-0.118100	0.536600

C	3.952200	1.125200	0.572600
H	1.986100	-2.094100	-0.363100
H	4.403700	-2.233800	0.169200
H	5.651500	-0.180300	0.767800
H	4.511300	2.016100	0.831400
H	2.102300	2.169800	0.306200

CP prod

C	3.003000	-0.851200	-0.230100
C	3.034100	0.232900	0.560700
C	1.894600	-1.838100	-0.189400
C	0.640300	-1.444500	0.514200
C	0.674000	-0.206100	1.409700
C	1.958900	0.539800	1.536200
C	-0.108500	-0.190000	0.109700
O	2.026900	-2.944700	-0.686600
O	2.136700	1.355500	2.426900
H	3.822300	-1.088500	-0.899900
H	3.880900	0.910700	0.560600
H	0.084200	-0.224400	2.317700
H	0.030000	-2.280400	0.832000
C	0.367800	0.610700	-1.092200
O	0.538300	0.140300	-2.192400
O	0.505300	1.903800	-0.789300
C	0.859100	2.793600	-1.877600
H	1.821800	2.504200	-2.297900
H	0.915200	3.782400	-1.431000
H	0.090500	2.760500	-2.649200
C	-1.617900	-0.203400	0.185700
C	-2.348100	-1.148100	-0.543200
C	-2.297800	0.756100	0.942600
C	-3.741200	-1.139100	-0.505500
H	-1.827400	-1.891200	-1.136300
C	-3.691200	0.762500	0.979700
H	-1.738600	1.495700	1.504100
C	-4.415300	-0.184500	0.256000
H	-4.298500	-1.878500	-1.069100
H	-4.209100	1.506300	1.574200
H	-5.498800	-0.179900	0.286600

For D(Me)

Benzoquinone(BQ)

C	-3.250300	1.089000	0.000000
C	-3.285700	-0.252700	0.000000
C	-1.950200	1.799400	0.000000
C	-0.689400	1.021400	0.000000
C	-0.724800	-0.320300	0.000000
C	-2.024900	-1.030800	0.000000
O	-1.918000	3.019400	0.000000
O	-2.057100	-2.250800	0.000000
H	0.266500	1.536700	0.000000
H	0.202500	-0.885400	0.000000
H	-4.241600	-0.768100	0.000000
H	-4.177600	1.654000	0.000000

CH_3 carbene

C	-2.694100	-0.849000	0.312500
C	-1.783000	-0.264000	-0.662100
C	-0.605800	0.398600	-0.167400
O	-0.685400	1.588700	0.118300
O	0.504600	-0.339900	-0.157200

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 C    1.764800    0.338400    0.151000
 C    2.871100   -0.685800    0.026500
 H    1.696200    0.745900    1.160600
 H    1.887600    1.163600   -0.552100
 H    2.723600   -1.510700    0.726900
 H    3.828200   -0.210000    0.254700
 H    2.921400   -1.088700   -0.987200
 H   -3.452200   -1.500700   -0.122500
 H   -3.234800    0.060400    0.652500
 H   -2.241200   -1.279000    1.215200
EPTS1
 C   -1.986000   -1.328800   -0.652700
 C   -3.319000   -1.202400   -0.594600
 C   -1.092000   -0.312000   -0.053800
 C   -1.719000    0.849600    0.614900
 C   -3.052200    0.974700    0.677200
 C   -3.950200   -0.039900    0.074100
 O   -5.167200    0.078600    0.129100
 H   -1.501800   -2.169200   -1.136600
 H   -3.991100   -1.934000   -1.028300
 H   -1.052000    1.578900    1.057800
 H   -3.533300    1.812600    1.168600
 C    3.138300    0.207100   -0.258000
 O    4.237300    0.611100   -0.639700
 O    2.942600   -0.885700    0.480600
 C    4.121100   -1.670300    0.786400
 H    4.831100   -1.082500    1.367800
 H    4.592700   -2.019300   -0.132300
 O    0.128000   -0.447700   -0.110100
 C    2.009900    0.940900   -0.759700
 C    1.659400    2.206400   -0.105200
 H    2.491000    2.864100   -0.417900
 H    0.745400    2.658700   -0.490900
 H    1.674400    2.201300    0.991900
 C    3.604500   -2.862300    1.613300
 H    2.889200   -3.412200    1.038000
 H    4.424000   -3.501300    1.868400
 H    3.141400   -2.501800    2.508000
EPINT
 C   -1.704100   -1.305600   -0.148300
 C   -3.040800   -1.565000   -0.105800
 C   -1.223300    0.026500   -0.037500
 C   -2.130600    1.107800    0.118900
 C   -3.471400    0.850100    0.160900
 C   -4.017500   -0.496900    0.050900
 O   -5.247400   -0.716200    0.090300
 H   -0.975900   -2.099700   -0.266700
 H   -3.413500   -2.579100   -0.189400
 H   -1.784100    2.125200    0.203700
 H   -4.178500    1.663000    0.278800
 C    2.399200    0.606300   -0.180900
 O    3.331200    1.389900   -0.145100
 O    2.510800   -0.714900   -0.346800
 C    3.854700   -1.267400   -0.481900
 H    4.467900   -0.556600   -1.034900
 H    3.707000   -2.163600   -1.082700
 O    0.120400    0.108100   -0.102800
 C    0.996000    1.063300   -0.048700
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C	0.684200	2.497600	0.128200
H	0.060500	2.872900	-0.691500
H	0.145700	2.673000	1.066600
H	1.615000	3.058900	0.146100
C	4.452800	-1.595800	0.874100
H	5.427200	-2.070600	0.729400
H	4.599000	-0.694900	1.473200
H	3.813300	-2.289400	1.424600

EPTS2

C	2.216800	0.617900	1.264200
C	3.404000	0.195400	0.744500
C	1.008900	0.123900	0.715300
C	1.014200	-0.836900	-0.332100
C	2.200100	-1.265100	-0.856900
C	3.470600	-0.758900	-0.368800
O	4.568300	-1.126100	-0.833900
H	2.171600	1.323700	2.085400
H	4.346500	0.548100	1.147100
H	0.070300	-1.247300	-0.670100
C	-1.988700	0.761600	-0.397000
O	-2.571000	1.372100	-1.275000
O	-2.444900	-0.334900	0.212800
C	-3.760600	-0.814600	-0.196700
H	-3.731500	-1.006600	-1.270900
H	-4.484100	-0.019300	-0.008500
O	-0.208600	0.573500	1.229600
C	-0.664600	1.190100	0.111100
C	-0.041100	2.423600	-0.440900
H	0.785600	2.755900	0.184900
H	0.330500	2.281600	-1.460900
H	-0.806000	3.205500	-0.493800
H	2.224500	-2.020900	-1.632500
C	-4.061800	-2.063500	0.601000
H	-5.044800	-2.444000	0.312400
H	-3.322300	-2.843200	0.405900
H	-4.077300	-1.852200	1.672300

EP prod

C	-0.796700	0.438800	-0.487400
C	-0.801900	-1.016900	-0.227400
C	-1.922100	-1.665800	0.120600
C	-3.219400	-0.972100	0.215500
O	0.180700	0.895300	-1.465800
C	1.572600	0.534300	0.590500
O	1.778300	0.688300	1.773800
O	2.297800	-0.231400	-0.219000
C	3.428300	-0.942600	0.377200
H	3.041700	-1.594800	1.162100
H	4.087900	-0.203600	0.834400
H	-1.919400	-2.729000	0.330900
H	0.140400	-1.542100	-0.324200
O	-4.240500	-1.555000	0.575700
C	0.434400	1.253800	-0.123300
C	0.363900	2.720900	0.243000
H	-0.410500	3.234800	-0.321600
H	0.172900	2.836600	1.310200
H	1.322300	3.194600	0.014200
C	-3.236800	0.449700	-0.176400
H	-4.202700	0.941500	-0.186000

C	-2.116800	1.100500	-0.523000
H	-2.155300	2.135300	-0.837500
C	4.113000	-1.717300	-0.726800
H	4.964400	-2.259800	-0.308300
H	3.434000	-2.443100	-1.179300
H	4.483300	-1.047900	-1.506100

MBQ

For A(X=H)

MBQ(Methyl benzoquinone)

C	1.029600	0.773800	-0.000100
C	0.798300	-0.710900	0.000000
C	-0.465300	-1.171600	0.000000
C	-1.649000	-0.284800	0.000000
C	-1.402800	1.180200	0.000000
C	-0.157100	1.666300	0.000000
O	-2.783200	-0.733900	0.000000
O	2.154600	1.242400	0.000100
C	2.010600	-1.599900	0.000000
H	-0.688700	-2.234000	0.000000
H	0.062200	2.728200	0.000000
H	-2.284400	1.811500	0.000000
H	2.919600	-1.000500	0.000000
H	2.017300	-2.246300	-0.881700
H	2.017300	-2.246300	0.881700

H carbene

C	-1.825500	-0.799000	0.000000
H	-2.629300	-0.040900	-0.000100
C	-0.568500	0.054400	0.000000
O	-0.529400	1.270100	0.000000
O	0.521900	-0.723300	0.000000
C	1.791700	-0.037400	0.000000
H	2.546200	-0.818600	0.000000
H	1.878400	0.588500	0.889500
H	1.878400	0.588500	-0.889500

EP INT

C	1.261700	-0.925600	0.000100
C	2.625100	-0.884400	0.000000
C	0.488200	0.266400	0.000100
C	1.099900	1.547300	0.000000
C	2.458000	1.617300	-0.000200
C	3.303700	0.421800	0.000000
O	4.543500	0.515200	0.000100
H	0.727900	-1.869800	0.000200
H	0.506600	2.452700	0.000000
H	2.966100	2.574300	-0.000200
C	-3.174200	0.456000	0.000000
O	-4.124300	1.224600	0.000100
O	-3.278700	-0.883000	0.000000
C	-4.619800	-1.418800	0.000000
H	-5.157000	-1.094500	-0.891600
H	-5.156800	-1.094800	0.891700
H	-4.496300	-2.498500	-0.000200
O	-0.833000	0.074300	0.000000

C	-1.807700	0.938700	0.000000
H	-1.614700	2.001600	-0.000300
C	3.473400	-2.120800	-0.000100
H	4.128100	-2.142500	-0.876300
H	4.128100	-2.142700	0.876200
H	2.857500	-3.021200	-0.000200

EP TS

C	1.489800	-1.849800	-0.272000
C	2.751900	-1.400400	-0.048400
C	0.437500	-0.901100	-0.359300
C	0.685800	0.499400	-0.265600
C	1.947400	0.979100	-0.057100
C	3.057700	0.031400	0.092700
O	4.223800	0.406300	0.298500
H	1.259400	-2.903400	-0.375200
H	3.588500	-2.085000	0.028700
H	-0.148100	1.176700	-0.412300
C	-2.635700	-0.147900	0.559100
O	-3.237800	0.119500	1.586600
O	-3.018400	0.221500	-0.672500
C	-4.255200	0.963000	-0.764400
H	-4.179000	1.892000	-0.199000
H	-5.082200	0.365000	-0.381200
H	-4.388800	1.167900	-1.823100
O	-0.846200	-1.361800	-0.594500
C	-1.409600	-0.931200	0.560700
H	-1.017400	-1.306500	1.495100
C	2.256300	2.446100	-0.000800
H	2.692300	2.713300	0.966700
H	2.994000	2.719600	-0.760800
H	1.356800	3.044100	-0.153900

EP prod

C	-2.444000	-1.410300	-0.222500
C	-1.216300	-1.837800	0.095900
C	-2.780800	0.026000	-0.261100
C	-1.722200	0.997900	0.131300
C	-0.493000	0.549800	0.443200
C	-0.132900	-0.879300	0.385200
O	-3.903900	0.402900	-0.586500
O	0.850600	-1.328500	1.359400
C	1.264900	-1.309400	0.013400
C	2.315800	-0.338700	-0.458100
O	2.765800	-0.400400	-1.580400
O	2.677000	0.547400	0.466600
C	3.688200	1.511600	0.079600
H	1.365500	-2.278500	-0.468500
C	-2.098800	2.450100	0.166900
H	-3.245800	-2.100400	-0.458000
H	-0.971100	-2.893500	0.139200
H	0.287800	1.235500	0.750800
H	-2.936100	2.616300	0.850200
H	-2.427600	2.787600	-0.819900
H	-1.256000	3.064400	0.485900
H	3.847100	2.126600	0.960800
H	3.329900	2.115000	-0.753900
H	4.605400	0.995500	-0.201700

For B(X=CO_2Me)

MBQ(Methyl benzoquinone)

C	1.029600	0.773800	-0.000100
C	0.798300	-0.710900	0.000000
C	-0.465300	-1.171600	0.000000
C	-1.649000	-0.284800	0.000000
C	-1.402800	1.180200	0.000000
C	-0.157100	1.666300	0.000000
O	-2.783200	-0.733900	0.000000
O	2.154600	1.242400	0.000100
C	2.010600	-1.599900	0.000000
H	-0.688700	-2.234000	0.000000
H	0.062200	2.728200	0.000000
H	-2.284400	1.811500	0.000000
H	2.919600	-1.000500	0.000000
H	2.017300	-2.246300	-0.881700
H	2.017300	-2.246300	0.881700

CO_2Me carbene

C	-1.255300	-0.333900	0.211100
C	0.000400	-0.374700	0.906100
C	1.255100	-0.337300	0.207200
O	-1.640100	-1.391000	-0.264800
O	1.640600	-1.390000	-0.276500
O	-1.898000	0.821600	0.230500
O	1.897700	0.818900	0.234200
C	-3.227700	0.846600	-0.364800
C	3.227300	0.848600	-0.360700
H	3.581000	1.862300	-0.198600
H	3.163100	0.627700	-1.425000
H	3.873100	0.128500	0.139600
H	-3.582300	1.860900	-0.208600
H	-3.872900	0.128800	0.139400
H	-3.162800	0.619800	-1.427800

EPINT

C	-1.672900	-1.788900	0.718800
C	-3.022800	-1.729600	0.723500
C	-0.916100	-0.703500	0.165600
C	-1.557100	0.396200	-0.473600
C	-2.914800	0.467500	-0.523100
C	-3.733500	-0.593600	0.127600
O	-4.964900	-0.529600	0.133500
H	-1.126900	-2.618500	1.151400
H	-3.627200	-2.515000	1.159900
H	-0.958600	1.152300	-0.960400
C	2.690200	-0.727200	-0.178600
O	3.780700	-0.190200	-0.228900
O	2.517300	-2.060100	-0.324100
C	3.719600	-2.835300	-0.504700
H	4.380300	-2.722600	0.355500
H	4.241500	-2.523600	-1.409800
H	3.384500	-3.865700	-0.594500
O	0.386600	-0.875100	0.248400
C	1.413000	-0.036300	0.026500
C	1.275500	1.383700	0.365800
O	2.274100	2.138200	-0.105700
O	0.359200	1.821300	1.044500
C	2.278700	3.522200	0.308500

H	3.151800	3.958100	-0.169800
H	1.368300	4.021400	-0.023900
H	2.362000	3.592100	1.393200
C	-3.639600	1.568500	-1.228100
H	-4.303600	1.163000	-1.996900
H	-4.277000	2.114600	-0.526200
H	-2.942800	2.267900	-1.690100

EPTS

C	-1.817700	-0.028300	-1.165800
C	-2.990100	-0.098600	-0.476200
C	-0.638500	-0.624500	-0.645000
C	-0.654400	-1.382900	0.576800
C	-1.804800	-1.481900	1.283800
C	-3.031200	-0.830000	0.831300
O	-4.081800	-0.895500	1.472400
H	-1.742600	0.500300	-2.107200
H	0.248200	-1.897300	0.878400
H	-1.864100	-2.067600	2.192600
C	2.516800	-0.509600	-0.012900
O	3.432400	0.035100	0.570400
O	2.529000	-1.809000	-0.374900
C	3.735600	-2.540900	-0.069600
H	3.919300	-2.537300	1.005000
H	4.586200	-2.098700	-0.588700
H	3.554800	-3.552200	-0.424400
O	0.510400	-0.542400	-1.382500
C	1.263800	0.136100	-0.439300
C	0.947900	1.569200	-0.255200
O	1.555700	2.094200	0.814700
O	0.217000	2.198900	-0.998300
C	1.361400	3.509200	1.031000
H	1.934100	3.741100	1.925100
H	1.735400	4.077000	0.179000
H	0.304300	3.727500	1.184000
C	-4.255600	0.520600	-0.964600
H	-5.038800	-0.237300	-1.061500
H	-4.625800	1.249500	-0.237100
H	-4.111200	1.014900	-1.924800

EP prod

C	-2.156400	-1.863800	0.357900
C	-0.928700	-1.539600	0.778100
C	-3.092400	-0.851200	-0.168500
C	-2.659500	0.573900	-0.136700
C	-1.423300	0.882300	0.292800
C	-0.444400	-0.145500	0.701500
O	-4.198600	-1.173500	-0.591400
O	0.497000	0.236000	1.745900
C	1.037100	0.076400	0.461300
C	1.555900	1.311700	-0.266600
O	2.177700	1.236500	-1.299600
O	1.264200	2.436500	0.376300
C	1.732000	3.667800	-0.233900
C	1.963000	-1.126700	0.278800
C	-3.653500	1.606000	-0.581000
H	-2.521000	-2.883500	0.397900
H	-0.257300	-2.284800	1.189400
H	-1.097800	1.913500	0.349000

H	-4.567200	1.545200	0.016300
H	-3.946200	1.435300	-1.620700
H	-3.239600	2.611000	-0.492800
H	1.406100	4.457400	0.437000
H	1.285600	3.786900	-1.220500
H	2.818100	3.651000	-0.314200
O	2.759800	-1.468400	1.117500
O	1.770700	-1.711500	-0.896900
C	2.642100	-2.825900	-1.220800
H	2.334600	-3.148300	-2.211300
H	2.508000	-3.626000	-0.493600
H	3.679800	-2.494000	-1.226200

For C(X=Ph)

MBQ(Methyl benzoquinone)

C	1.029600	0.773800	-0.000100
C	0.798300	-0.710900	0.000000
C	-0.465300	-1.171600	0.000000
C	-1.649000	-0.284800	0.000000
C	-1.402800	1.180200	0.000000
C	-0.157100	1.666300	0.000000
O	-2.783200	-0.733900	0.000000
O	2.154600	1.242400	0.000100
C	2.010600	-1.599900	0.000000
H	-0.688700	-2.234000	0.000000
H	0.062200	2.728200	0.000000
H	-2.284400	1.811500	0.000000
H	2.919600	-1.000500	0.000000
H	2.017300	-2.246300	-0.881700
H	2.017300	-2.246300	0.881700

Ph carbene

C	0.538000	-1.109100	0.003900
C	1.745600	-0.387500	0.282800
C	-0.722700	-0.471000	-0.000400
C	-0.905000	0.931200	0.187500
C	-1.876600	-1.274100	-0.221400
C	-2.169000	1.489400	0.153200
C	-3.283000	0.668900	-0.071600
C	-3.140400	-0.709400	-0.260000
O	2.169300	-0.289900	1.431400
O	2.410700	0.042000	-0.807300
C	3.737000	0.577700	-0.589900
H	4.107700	0.831200	-1.580000
H	4.377300	-0.171800	-0.124200
H	3.692800	1.467400	0.038200
H	-1.734300	-2.338800	-0.360000
H	-4.272400	1.111700	-0.099100
H	-4.014000	-1.326200	-0.431400
H	-0.038800	1.558700	0.361900
H	-2.303200	2.554700	0.296800

CHTS1/CPTS1

C	2.384200	-1.280600	0.597900
C	3.049400	-0.304700	-0.053400
C	1.158600	-1.851600	-0.038700
C	0.565000	-1.071500	-1.159500
C	1.301400	-0.142200	-1.841600
C	2.603000	0.279500	-1.338000
O	0.702900	-2.935700	0.297600

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 O    3.320200    1.079900   -1.947900
 H    3.982100    0.089800    0.338300
 H   -0.314700   -1.507400   -1.613600
 C   -0.619800    0.097900    0.319400
 C   -0.047600    1.323600    0.833800
 C   -2.012200   -0.016200    0.058000
 O   -0.204900    1.577700    2.023700
 O    0.690000    2.064500   -0.002600
 C    1.376300    3.200600    0.579600
 H    1.954100    3.628200   -0.235500
 H    2.032100    2.874600    1.386400
 H    0.653100    3.923000    0.957700
 C   -2.583100   -1.309600   -0.091800
 C   -2.874800    1.113400   -0.004200
 C   -3.944400   -1.462500   -0.287800
 C   -4.768400   -0.332900   -0.345600
 C   -4.234900    0.953000   -0.202400
 H   -1.935600   -2.175700   -0.029400
 H   -4.373400   -2.451600   -0.390800
 H   -5.834300   -0.455000   -0.501300
 H   -4.885200    1.817900   -0.249400
 H   -2.458000    2.107500    0.105000
 C    2.858300   -1.903700    1.875000
 H    2.094600   -1.816500    2.653300
 H    3.041000   -2.972500    1.733600
 H    3.775700   -1.430000    2.225100
 H    0.936400    0.320700   -2.750300
CHTS2
 C   -3.323900    0.194600   -0.155900
 C   -3.557100   -1.102200    0.110200
 C   -1.921500    0.641400   -0.320600
 C   -0.794400   -0.282800    0.214200
 C   -1.135500   -1.667400    0.317100
 C   -2.484700   -2.112200    0.305200
 O   -1.644800    1.672100   -0.898900
 O   -2.811200   -3.306900    0.476200
 H   -4.571700   -1.481700    0.181800
 H   -0.507600    0.036100    1.317300
 H   -0.377900   -2.406500    0.539000
 C    0.569000    0.268800    0.158000
 C    0.696400    1.743200    0.416300
 C    1.776700   -0.528700    0.049300
 O    0.152700    2.325200    1.332500
 O    1.514100    2.318500   -0.467800
 C    1.724700    3.742900   -0.318400
 H    2.150500    3.959100    0.661400
 H    0.780300    4.273100   -0.438100
 H    2.419800    4.012600   -1.108800
 C    1.807500   -1.694500   -0.746800
 C    2.973100   -0.113300    0.676600
 C    2.992700   -2.391900   -0.932500
 C    4.162900   -1.972100   -0.296100
 C    4.147200   -0.832900    0.512100
 H    0.907100   -2.035300   -1.241000
 H    3.004100   -3.270500   -1.566600
 H    5.081600   -2.532100   -0.426300
 H    5.052400   -0.507200    1.010500
 H    2.975300    0.772400    1.300300
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 C   -4.398500    1.216100   -0.390000
 H   -4.286700    2.063000    0.293100
 H   -4.336200    1.617200   -1.405000
 H   -5.385100    0.775300   -0.244900
CP prod
 C    1.479200   -1.668500   -1.027800
 C    2.868400   -1.564000   -0.451100
 C    0.847600   -0.311700   -0.900900
 C    3.281300   -0.553500    0.354500
 C    2.301200    0.548300    0.780900
 C    0.920400    0.007200    0.589800
 C   -0.338800    0.332600   -0.213700
 C   -0.531100    1.789500   -0.616000
 C    4.682800   -0.429300    0.867000
 O    1.015300   -2.701000   -1.464700
 O    2.662700    1.645800    1.142800
 H    5.320400   -1.225800    0.483600
 H    4.699500   -0.455900    1.961100
 H    5.102200    0.537200    0.572500
 H    3.550400   -2.366400   -0.715700
 H    1.391200    0.422800   -1.488600
 H    0.764800   -0.880600    1.196200
 O    0.223500    2.408100   -1.332500
 O   -1.623000    2.307300   -0.053000
 C   -1.887800    3.705500   -0.319300
 H   -2.024900    3.863200   -1.388800
 H   -2.802500    3.930300    0.222400
 H   -1.063400    4.318600    0.044000
 C   -1.578400   -0.447400    0.136000
 C   -2.313500   -1.061400   -0.882900
 C   -2.025000   -0.546600    1.456400
 C   -3.481200   -1.761300   -0.585000
 H   -1.967900   -0.996800   -1.908600
 C   -3.191600   -1.248700    1.754600
 H   -1.462500   -0.071300    2.252300
 C   -3.923100   -1.856300    0.734500
 H   -4.041000   -2.236700   -1.382300
 H   -3.527700   -1.321000    2.782800
 H   -4.829100   -2.404400    0.966700

CH prod
 C   -3.600400   -0.197300   -0.034900
 C   -3.180800    0.978700    0.464800
 C   -2.576000   -1.237500   -0.369400
 C   -1.147100   -0.925800   -0.145100
 C   -0.736000    0.251900    0.348100
 C   -1.758400    1.286600    0.699100
 O   -2.908800   -2.325000   -0.822100
 O   -1.415100    2.361200    1.177400
 C   -5.037200   -0.536100   -0.277300
 H   -5.685800    0.293100    0.004600
 H   -5.324300   -1.423200    0.294100
 H   -5.202800   -0.775200   -1.331600
 H   -3.878500    1.766400    0.728400
 C    0.704400    0.593700    0.592800
 C    1.221300    1.683200   -0.333500
 O    0.734100    1.980400   -1.400900
 O    2.323800    2.251400    0.170700
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C	2.961400	3.266800	-0.639600
H	3.821300	3.596200	-0.062500
H	2.275000	4.095500	-0.811600
H	3.278800	2.843300	-1.592500
H	0.854800	0.917400	1.624800
H	-0.449400	-1.713100	-0.409500
C	1.587700	-0.648400	0.372300
C	2.062700	-1.369900	1.467800
C	1.912700	-1.052200	-0.922700
C	2.863200	-2.494500	1.268400
H	1.807000	-1.050900	2.488600
C	2.712500	-2.177700	-1.122300
H	1.538200	-0.483800	-1.786300
C	3.187900	-2.898800	-0.027100
H	3.238100	-3.062900	2.131900
H	2.968300	-2.496100	-2.143500
H	3.819000	-3.785600	-0.184100

For D(X=Me)

MBQ(Methyl benzoquinone)

C	1.029600	0.773800	-0.000100
C	0.798300	-0.710900	0.000000
C	-0.465300	-1.171600	0.000000
C	-1.649000	-0.284800	0.000000
C	-1.402800	1.180200	0.000000
C	-0.157100	1.666300	0.000000
O	-2.783200	-0.733900	0.000000
O	2.154600	1.242400	0.000100
C	2.010600	-1.599900	0.000000
H	-0.688700	-2.234000	0.000000
H	0.062200	2.728200	0.000000
H	-2.284400	1.811500	0.000000
H	2.919600	-1.000500	0.000000
H	2.017300	-2.246300	-0.881700
H	2.017300	-2.246300	0.881700

CH_3 carbene

C	-2.694100	-0.849000	0.312500
C	-1.783000	-0.264000	-0.662100
C	-0.605800	0.398600	-0.167400
O	-0.685400	1.588700	0.118300
O	0.504600	-0.339900	-0.157200
C	1.764800	0.338400	0.151000
C	2.871100	-0.685800	0.026500
H	1.696200	0.745900	1.160600
H	1.887600	1.163600	-0.552100
H	2.723600	-1.510700	0.726900
H	3.828200	-0.210000	0.254700
H	2.921400	-1.088700	-0.987200
H	-3.452200	-1.500700	-0.122500
H	-3.234800	0.060400	0.652500
H	-2.241200	-1.279000	1.215200

EPTS1

C	-1.613400	-1.716800	-0.204000
C	-2.934200	-1.894200	-0.329900

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 C   -1.057600   -0.384100    0.121100
 C   -1.998900    0.732500    0.304300
 C   -3.332300    0.582200    0.184600
 C   -3.883800   -0.771200   -0.150100
 O   -5.088200   -0.947500   -0.270800
 H   -0.899700   -2.521900   -0.334500
 H   -3.372700   -2.855900   -0.570400
 H   -1.561800    1.692600    0.553100
 C    3.022200    0.748900   -0.242400
 O    4.012900    1.281400   -0.748100
 O    3.044900   -0.301700    0.577100
 C    4.336100   -0.941300    0.819000
 H    5.114900   -0.179700    0.812300
 H    4.240600   -1.347700    1.825100
 O    0.159500   -0.238300    0.236300
 C    1.767400    1.287100   -0.689200
 C    4.602200   -2.032100   -0.202300
 H    4.689500   -1.618200   -1.208900
 H    5.542000   -2.535200    0.042100
 H    3.803100   -2.776700   -0.194600
 C    1.307000    2.547400   -0.088500
 H    2.051300    3.277000   -0.452800
 H    0.334200    2.876200   -0.453600
 H    1.355000    2.590300    1.006800
 C   -4.313900    1.695700    0.371900
 H   -4.909600    1.838000   -0.534100
 H   -5.018000    1.455800    1.173500
 H   -3.805400    2.629000    0.612900
EPINT
 C    1.890700    1.204100    0.332700
 C    3.015500    0.425800    0.303400
 C    0.658600    0.737400   -0.188800
 C    0.569100   -0.510000   -0.844700
 C    1.685700   -1.290600   -0.920800
 C    2.957500   -0.898300   -0.327400
 O    3.959800   -1.643400   -0.384200
 H   -0.349800   -0.817600   -1.322400
 H    1.664700   -2.231600   -1.458300
 C   -2.479700    0.343800    0.041100
 O   -3.669900    0.349100   -0.222300
 O   -1.836600   -0.653500    0.659000
 C   -2.618900   -1.819100    1.066200
 H   -3.592400   -1.475200    1.414700
 H   -2.054800   -2.223200    1.905100
 O   -0.355000    1.629100   -0.089000
 C   -1.657100    1.549500   -0.180200
 C   -2.339500    2.852900   -0.396900
 H   -2.664700    2.942400   -1.441500
 H   -3.233000    2.939400    0.223100
 H   -1.650500    3.670500   -0.184900
 C    4.322200    0.879100    0.885700
 H    4.239300    1.881600    1.308800
 H    4.657300    0.194900    1.671400
 H    5.108300    0.883100    0.124400
 H    1.906300    2.189200    0.786900
 C   -2.747200   -2.828900   -0.059900
 H   -3.287800   -3.704200    0.310700
 H   -3.305700   -2.417000   -0.902400
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 H   -1.765300   -3.157400   -0.406400
EPTS2
 C    1.930100   -1.313600   -1.185500
 C    3.164200   -0.853600   -0.838700
 C    0.791400   -0.586400   -0.764200
 C    0.916700    0.627300   -0.034400
 C    2.145000    1.112200    0.325700
 C    3.348400    0.365200   -0.045400
 O    4.492100    0.754100    0.263900
 H    1.795800   -2.216100   -1.770000
 H    4.063400   -1.374300   -1.147300
 H    0.014600    1.181800    0.198900
 C   -2.175900   -0.648000    0.568200
 O   -2.752900   -0.936500    1.602300
 O   -2.589100    0.270500   -0.311200
 C   -3.843100    0.949900   -0.009100
 H   -3.740500    1.435800    0.963100
 H   -4.628900    0.195800    0.064600
 O   -0.476300   -1.061200   -1.102300
 C   -0.920200   -1.310100    0.158100
 C    2.313800    2.407700    1.065000
 H    2.816700    2.246000    2.023500
 H    2.940900    3.102900    0.499100
 H    1.349400    2.881600    1.255100
 C   -0.359300   -2.396200    1.008300
 H    0.397600   -2.961700    0.466400
 H    0.089400   -2.014800    1.931400
 H   -1.175500   -3.061000    1.309500
 C   -4.105800    1.942300   -1.119900
 H   -5.043000    2.467000   -0.917700
 H   -3.305800    2.683100   -1.183500
 H   -4.196900    1.438300   -2.084500
EP prod
 C    0.579200   -0.764300   -0.490900
 C    0.744500    0.692200   -0.300000
 C    1.920300    1.259700    0.019300
 C    3.136200    0.411200    0.145500
 O   -0.445200   -1.158500   -1.448500
 C   -1.790000   -0.575000    0.586700
 O   -2.068200   -0.713300    1.755200
 O   -2.372800    0.293900   -0.238700
 C   -3.414800    1.139100    0.337600
 H   -2.969100    1.733100    1.137400
 H   -4.174600    0.489800    0.775400
 H   -0.144400    1.298300   -0.425200
 O    4.217900    0.885900    0.476100
 C   -0.729600   -1.431300   -0.092700
 C   -0.810200   -2.881000    0.336200
 H   -0.073900   -3.492700   -0.179300
 H   -0.662600   -2.963200    1.413100
 H   -1.803000   -3.271700    0.097900
 C    2.996500   -1.021200   -0.179600
 H    3.909200   -1.605600   -0.162600
 C    1.817000   -1.567800   -0.499600
 H    1.743900   -2.613300   -0.768800
 C    2.090800    2.733500    0.246300
 H    2.471600    2.925300    1.253300
 H    2.825400    3.149700   -0.448700
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H	1.146200	3.263900	0.120500
C	-3.969000	1.998900	-0.776900
H	-4.386900	1.381300	-1.574500
H	-4.764800	2.635100	-0.382000
H	-3.194700	2.641600	-1.200800

NQ

For A(X=H)
NQ(Naphthaquinone)

C	-2.675400	0.698100	0.000000
C	-2.675400	-0.698000	0.000000
C	-1.471600	1.396500	0.000000
C	-0.260000	0.703700	0.000000
C	-0.260100	-0.703700	0.000000
C	-1.471600	-1.396400	0.000000
C	1.024300	1.460300	0.000000
C	2.278400	0.669700	0.000000
C	2.278300	-0.669800	0.000000
C	1.024200	-1.460400	0.000100
O	1.062100	2.681800	0.000000
O	1.062000	-2.681900	0.000000
H	-1.452500	2.479100	0.000000
H	-1.452700	-2.479100	0.000000
H	3.196700	-1.246100	0.000000
H	3.196800	1.246000	0.000000
H	-3.613600	1.240200	0.000000
H	-3.613700	-1.240100	0.000000

H carbene

C	-1.825500	-0.799000	0.000000
H	-2.629300	-0.040900	-0.000100
C	-0.568500	0.054400	0.000000
O	-0.529400	1.270100	0.000000
O	0.521900	-0.723300	0.000000
C	1.791700	-0.037400	0.000000
H	2.546200	-0.818600	0.000000
H	1.878400	0.588500	0.889500
H	1.878400	0.588500	-0.889500

EPINT

C	-1.349300	-0.564600	0.000100
C	-2.358500	0.429400	0.000000
C	0.039100	-0.143600	0.000500
C	0.385400	1.233900	0.001000
C	-0.582900	2.190100	0.001000
C	-2.004900	1.869300	0.000400
O	-2.866800	2.757600	0.000200
H	1.429000	1.504100	0.001400
H	-0.318900	3.241000	0.001400
C	3.395700	-0.720300	0.000300
O	4.473200	-1.300000	0.001000
O	3.276200	0.618900	-0.001100
C	4.509200	1.375200	-0.001900
H	5.091600	1.142900	-0.893100
H	5.090600	1.146000	0.890800
H	4.204500	2.418500	-0.003800
O	0.900600	-1.144300	0.000600
C	2.166500	-1.488200	0.000800
H	2.284500	-2.561700	0.001300
C	-3.707000	0.046900	-0.000500

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 C   -4.063400   -1.292600   -0.000800
 C   -3.065700   -2.277100   -0.000700
 C   -1.726600   -1.921800   -0.000200
 H   -4.460400    0.824800   -0.000600
 H   -0.963700   -2.689400   -0.000100
 H   -5.108600   -1.578600   -0.001200
 H   -3.340500   -3.325600   -0.000900
EPTS
 C    1.200100   -2.203500   -0.518400
 C    2.515400   -2.039300   -0.205200
 C    0.298600   -1.115900   -0.459000
 C    0.757900    0.238300   -0.223500
 C    2.131200    0.418300    0.087900
 C    3.054800   -0.734900    0.174600
 O    4.238200   -0.611900    0.514700
 H    0.800000   -3.176800   -0.778400
 H    3.205500   -2.874300   -0.217100
 C   -2.850300   -0.463300    0.602500
 O   -3.454100   -0.378900    1.662200
 O   -3.272100    0.066600   -0.559900
 C   -4.555400    0.729100   -0.534400
 H   -5.337500    0.024100   -0.251800
 H   -4.712900    1.089300   -1.547400
 H   -4.536700    1.560000    0.171200
 O   -1.026700   -1.414400   -0.724000
 C   -1.599600   -1.181400    0.481900
 H   -1.172300   -1.659000    1.351500
 C    2.643100    1.715800    0.255900
 C    1.832300    2.823700    0.092900
 C    0.483300    2.649100   -0.259700
 C   -0.047900    1.383200   -0.411300
 H   -1.089400    1.272000   -0.682700
 H    3.693200    1.822300    0.498200
 H    2.235900    3.820900    0.220900
 H   -0.150700    3.514400   -0.414700
EP prod
 C   -2.910300   -2.190600    0.027600
 C   -3.824500   -1.195900   -0.329600
 C   -1.586900   -1.863700    0.301500
 C   -1.158500   -0.536000    0.223800
 C   -2.084200    0.469800   -0.105000
 C   -3.411600    0.126900   -0.389600
 C    0.267000   -0.166900    0.477500
 C    0.561900    1.267100    0.674600
 C   -0.332400    2.219700    0.383400
 C   -1.689600    1.906900   -0.099900
 O    1.028600   -1.082900    1.293000
 C    2.688400   -0.570600   -0.550600
 O    3.049100   -0.721800   -1.693900
 O    3.402700    0.019000    0.409100
 C    4.704800    0.517300    0.017100
 H    5.139300    0.928000    0.924100
 H    4.597200    1.289800   -0.744300
 H    5.315700   -0.298000   -0.369300
 H   -3.231600   -3.223400    0.095800
 H   -0.887100   -2.636800    0.593900
 H   -4.853500   -1.455800   -0.547600
 H   -4.102800    0.920600   -0.644200
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H	-0.096100	3.271600	0.493700
H	1.553100	1.511600	1.034800
O	-2.461500	2.795000	-0.440000
C	1.344600	-1.062500	-0.083300
H	1.001600	-1.911500	-0.667900

For B(X=CO2Me)

NQ(Naphthaquinone)

C	-2.675400	0.698100	0.000000
C	-2.675400	-0.698000	0.000000
C	-1.471600	1.396500	0.000000
C	-0.260000	0.703700	0.000000
C	-0.260100	-0.703700	0.000000
C	-1.471600	-1.396400	0.000000
C	1.024300	1.460300	0.000000
C	2.278400	0.669700	0.000000
C	2.278300	-0.669800	0.000000
C	1.024200	-1.460400	0.000100
O	1.062100	2.681800	0.000000
O	1.062000	-2.681900	0.000000
H	-1.452500	2.479100	0.000000
H	-1.452700	-2.479100	0.000000
H	3.196700	-1.246100	0.000000
H	3.196800	1.246000	0.000000
H	-3.613600	1.240200	0.000000
H	-3.613700	-1.240100	0.000000

CO_2Me carbene

C	-1.255300	-0.333900	0.211100
C	0.000400	-0.374700	0.906100
C	1.255100	-0.337300	0.207200
O	-1.640100	-1.391000	-0.264800
O	1.640600	-1.390000	-0.276500
O	-1.898000	0.821600	0.230500
O	1.897700	0.818900	0.234200
C	-3.227700	0.846600	-0.364800
C	3.227300	0.848600	-0.360700
H	3.581000	1.862300	-0.198600
H	3.163100	0.627700	-1.425000
H	3.873100	0.128500	0.139600
H	-3.582300	1.860900	-0.208600
H	-3.872900	0.128800	0.139400
H	-3.162800	0.619800	-1.427800

EPINT

C	-1.739500	-0.711200	0.067900
C	-2.997700	-0.116900	-0.193600
C	-0.544800	-0.009900	-0.345500
C	-0.617000	1.213900	-1.084400
C	-1.814100	1.771700	-1.369900
C	-3.082200	1.182700	-0.908800
O	-4.153700	1.735700	-1.144500
H	0.300600	1.641300	-1.467600
H	-1.887200	2.661200	-1.983800
C	2.120200	1.260600	0.453500
O	3.188700	1.841000	0.396800
O	1.044800	1.771200	1.108400
C	1.217800	3.067500	1.715200
H	1.501500	3.805400	0.964300
H	1.980200	3.025000	2.493300

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 H    0.250100    3.314800    2.144900
 O    0.587500   -0.598900   -0.067700
 C    1.846000   -0.060400   -0.095900
 C   -4.163400   -0.761300    0.223300
 C   -4.094100   -1.983700    0.884100
 C   -2.851900   -2.570700    1.144400
 C   -1.680500   -1.937800    0.752100
 H   -5.118000   -0.292900    0.019500
 H   -0.718800   -2.382000    0.972200
 C    2.823600   -1.099100   -0.393800
 O    4.101100   -0.694500   -0.274000
 C    5.106200   -1.680900   -0.580500
 H    6.056400   -1.167200   -0.455600
 H    5.036800   -2.525100    0.106300
 H    4.995900   -2.035100   -1.606000
 O    2.510600   -2.233400   -0.726400
 H   -5.004100   -2.479400    1.200100
 H   -2.799400   -3.520800    1.662300
EPTS
 C    1.215000   -1.357500   -1.687500
 C    2.435400   -1.709000   -1.224000
 C    0.511700   -0.243100   -1.128700
 C    1.194700    0.705000   -0.262100
 C    2.474300    0.346100    0.231700
 C    3.108400   -0.935600   -0.164800
 O    4.168300   -1.327800    0.315800
 H    0.697100   -1.941000   -2.436200
 H    2.957000   -2.581700   -1.598100
 C   -2.440100    0.720000   -0.003100
 O   -3.214100    0.659200    0.933600
 O   -2.409200    1.770900   -0.860000
 C   -3.395200    2.798800   -0.632400
 H   -4.400700    2.387100   -0.723600
 H   -3.217100    3.543400   -1.404400
 H   -3.268600    3.235600    0.358700
 O   -0.763000   -0.072800   -1.574300
 C   -1.462000   -0.299400   -0.384100
 C    3.188300    1.240400    1.034500
 C    2.669800    2.495500    1.324500
 C    1.432400    2.874800    0.791800
 C    0.700000    1.994300    0.011200
 H   -0.252400    2.300000   -0.398100
 H    4.161000    0.940500    1.403700
 C   -1.470100   -1.684900    0.107700
 O   -1.015400   -2.635200   -0.510800
 O   -2.050200   -1.807100    1.311700
 C   -2.171200   -3.149800    1.826200
 H   -2.783400   -3.759300    1.161000
 H   -1.187000   -3.605400    1.938800
 H   -2.654800   -3.040400    2.793700
 H    3.230500    3.185800    1.943100
 H    1.039700    3.865400    0.987700
EP prod
 C   -2.817000    2.034500   -0.700100
 C   -3.859900    1.341400   -0.082900
 C   -1.579300    1.426100   -0.885800
 C   -1.369600    0.113600   -0.457300
 C   -2.434600   -0.602500    0.117900
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C	-3.668600	0.025900	0.316000
C	-0.043000	-0.559300	-0.616400
C	-0.051900	-2.040100	-0.573500
C	-1.080100	-2.721000	-0.054800
C	-2.299700	-2.051900	0.437200
O	0.876900	0.055300	-1.542800
C	2.461000	-0.608200	0.292700
O	2.942200	-0.440300	1.386000
O	2.937900	-1.429700	-0.639300
C	4.123400	-2.181300	-0.275400
H	4.371100	-2.765900	-1.156600
H	3.908000	-2.829700	0.573500
H	4.933100	-1.497700	-0.023000
H	-2.968800	3.051400	-1.042600
H	-0.779100	1.964200	-1.377400
H	-4.819200	1.822000	0.067600
H	-4.469000	-0.546500	0.768000
H	-1.060700	-3.801400	0.026700
H	0.835500	-2.542200	-0.935500
O	-3.175200	-2.676800	1.020800
C	1.225700	0.149400	-0.180100
C	1.125000	1.502400	0.520500
O	1.607200	2.470000	-0.260400
O	0.702000	1.643700	1.636900
C	1.612600	3.803600	0.308000
H	2.208400	3.816800	1.220100
H	2.057000	4.437100	-0.454100
H	0.592800	4.119100	0.527500

For C(X=Ph)

NQ(Naphthaquinone)

C	-2.675400	0.698100	0.000000
C	-2.675400	-0.698000	0.000000
C	-1.471600	1.396500	0.000000
C	-0.260000	0.703700	0.000000
C	-0.260100	-0.703700	0.000000
C	-1.471600	-1.396400	0.000000
C	1.024300	1.460300	0.000000
C	2.278400	0.669700	0.000000
C	2.278300	-0.669800	0.000000
C	1.024200	-1.460400	0.000100
O	1.062100	2.681800	0.000000
O	1.062000	-2.681900	0.000000
H	-1.452500	2.479100	0.000000
H	-1.452700	-2.479100	0.000000
H	3.196700	-1.246100	0.000000
H	3.196800	1.246000	0.000000
H	-3.613600	1.240200	0.000000
H	-3.613700	-1.240100	0.000000

Ph carbene

C	0.538000	-1.109100	0.003900
C	1.745600	-0.387500	0.282800
C	-0.722700	-0.471000	-0.000400
C	-0.905000	0.931200	0.187500
C	-1.876600	-1.274100	-0.221400
C	-2.169000	1.489400	0.153200
C	-3.283000	0.668900	-0.071600
C	-3.140400	-0.709400	-0.260000
O	2.169300	-0.289900	1.431400

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 O    2.410700    0.042000   -0.807300
 C    3.737000    0.577700   -0.589900
 H    4.107700    0.831200   -1.580000
 H    4.377300   -0.171800   -0.124200
 H    3.692800    1.467400    0.038200
 H   -1.734300   -2.338800   -0.360000
 H   -4.272400    1.111700   -0.099100
 H   -4.014000   -1.326200   -0.431400
 H   -0.038800    1.558700    0.361900
 H   -2.303200    2.554700    0.296800
CHTS1/CPTS1
 C   -0.980900   -1.962400   -0.716200
 C    0.097200   -2.001200    0.308800
 C   -0.060100   -1.418400    1.528800
 C   -1.202400   -0.555800    1.838800
 O   -0.921300   -2.671700   -1.709600
 O   -1.299600   -0.003400    2.933400
 H    0.887800   -2.716600    0.130700
 C    1.586900   -0.342500   -0.487500
 C    2.851900   -0.820600    0.050400
 O    3.862200   -0.351900   -0.726700
 O    3.021800   -1.617100    0.959300
 C    5.164400   -0.942300   -0.513700
 H    5.125500   -2.019500   -0.678500
 H    5.814900   -0.469200   -1.245100
 H    5.514700   -0.737400    0.498000
 H    0.681500   -1.547100    2.307100
 C   -2.241800   -0.382500    0.780600
 C   -2.136100   -1.060600   -0.450100
 C   -3.131800   -0.903000   -1.418500
 C   -3.340600    0.447100    1.018200
 C   -4.323400    0.603900    0.045800
 C   -4.219700   -0.071600   -1.173100
 H   -3.412300    0.959200    1.969500
 H   -3.039000   -1.436300   -2.356400
 C    1.193500    1.021500   -0.381200
 C    0.169900    1.499500   -1.241500
 C    1.827600    1.950900    0.489200
 C   -0.188600    2.838100   -1.244700
 H   -0.303800    0.800800   -1.918900
 C    1.456200    3.283700    0.492300
 H    2.605500    1.603700    1.158900
 C    0.450100    3.726400   -0.375400
 H   -0.958400    3.196100   -1.917300
 H    1.941300    3.984500    1.160900
 H    0.165700    4.772700   -0.374000
 H   -5.173000    1.249400    0.236200
 H   -4.988100    0.050100   -1.927500
CHINT
 C   -4.994200    0.937900   -0.224400
 C   -5.302700   -0.421600   -0.124900
 C   -3.670100    1.356000   -0.177500
 C   -2.641400    0.418700   -0.031700
 C   -2.953400   -0.948500    0.068400
 C   -4.286900   -1.359600    0.022000
 C   -1.234200    0.895000    0.011300
 C   -0.141100   -0.135200    0.136500
 C   -0.504100   -1.478700    0.269900
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 C   -1.871600   -1.957600    0.239600
 O   -0.966700    2.083900   -0.067200
 O   -2.122700   -3.159900    0.360500
 C    1.190100    0.303300    0.145600
 C    1.526800    1.760800    0.353400
 O    1.613700    2.265100    1.448600
 O    1.854500    2.355000   -0.795000
 C    2.207400    3.755200   -0.708600
 H    2.444900    4.054600   -1.725800
 H    3.069800    3.889500   -0.055800
 H    1.361400    4.327100   -0.327000
 C    2.359800   -0.572300    0.022000
 C    2.382000   -1.641700   -0.895900
 C    3.518000   -0.320300    0.785200
 C    3.514300   -2.435700   -1.030500
 C    4.643300   -2.189400   -0.249300
 C    4.639500   -1.129500    0.658100
 H   -5.787500    1.667200   -0.338200
 H   -6.336100   -0.746100   -0.161200
 H   -3.412400    2.404600   -0.252900
 H   -4.506200   -2.416600    0.104500
 H    3.521600    0.495300    1.497700
 H    5.513500   -0.932200    1.267500
 H    5.523100   -2.813600   -0.353200
 H    3.518100   -3.243500   -1.752900
 H    1.524800   -1.820000   -1.532400
 H    0.245700   -2.239800    0.439700
CHTS2
 C   -2.650600    0.470300   -0.230700
 C   -2.974700   -0.812500    0.006400
 C   -1.218800    0.824900   -0.363000
 C   -0.165800   -0.182300    0.172900
 C   -0.600400   -1.542500    0.243500
 C   -1.975800   -1.895600    0.200300
 O   -0.863400    1.845100   -0.916400
 O   -2.384400   -3.068500    0.342700
 H    0.121900    0.096900    1.286500
 H    0.102000   -2.334700    0.464000
 C    1.232300    0.277400    0.150200
 C    1.453200    1.735100    0.438800
 C    2.385700   -0.597300    0.046900
 O    0.933300    2.335700    1.356800
 O    2.323300    2.270000   -0.420400
 C    2.625900    3.674100   -0.240200
 H    3.047600    3.843500    0.750500
 H    1.721400    4.268600   -0.365500
 H    3.351500    3.910600   -1.013600
 C    2.353200   -1.748100   -0.770700
 C    3.595600   -0.274400    0.702100
 C    3.492300   -2.520000   -0.949500
 C    4.676100   -2.191100   -0.285400
 C    4.721800   -1.068100    0.544000
 H    1.441100   -2.018800   -1.286500
 H    3.456600   -3.385900   -1.599800
 H    5.557600   -2.809100   -0.410600
 H    5.637500   -0.812800    1.063700
 H    3.645600    0.597900    1.342600
 C   -3.676200    1.594000   -0.469500
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 H   -3.589900    1.947800   -1.475600
 C   -5.097900    1.049400   -0.237100
 C   -5.296100   -0.407600    0.220700
 H   -6.283900   -0.786000    0.382100
 C   -4.223900   -1.212100    0.419800
 H   -4.367900   -2.223500    0.737900
 H   -5.846300    1.604200   -0.374000
CHprod
 C   -4.994200    0.937900   -0.224400
 C   -5.302700   -0.421600   -0.124900
 C   -3.670100    1.356000   -0.177500
 C   -2.641400    0.418700   -0.031700
 C   -2.953400   -0.948500    0.068400
 C   -4.286900   -1.359600    0.022000
 C   -1.234200    0.895000    0.011300
 C   -0.141100   -0.135200    0.136500
 C   -0.504100   -1.478700    0.269900
 C   -1.871600   -1.957600    0.239600
 O   -0.966700    2.083900   -0.067200
 O   -2.122700   -3.159900    0.360500
 C    1.190100    0.303300    0.145600
 C    1.526800    1.760800    0.353400
 O    1.613700    2.265100    1.448600
 O    1.854500    2.355000   -0.795000
 C    2.207400    3.755200   -0.708600
 H    2.444900    4.054600   -1.725800
 H    3.069800    3.889500   -0.055800
 H    1.361400    4.327100   -0.327000
 C    2.359800   -0.572300    0.022000
 C    2.382000   -1.641700   -0.895900
 C    3.518000   -0.320300    0.785200
 C    3.514300   -2.435700   -1.030500
 C    4.643300   -2.189400   -0.249300
 C    4.639500   -1.129500    0.658100
 H   -5.787500    1.667200   -0.338200
 H   -6.336100   -0.746100   -0.161200
 H   -3.412400    2.404600   -0.252900
 H   -4.506200   -2.416600    0.104500
 H    3.521600    0.495300    1.497700
 H    5.513500   -0.932200    1.267500
 H    5.523100   -2.813600   -0.353200
 H    3.518100   -3.243500   -1.752900
 H    1.524800   -1.820000   -1.532400
 H    0.245700   -2.239800    0.439700
CP prod
 C   -4.954300   -1.133200    0.196200
 C   -5.092100    0.026400   -0.565300
 C   -3.696800   -1.525100    0.650900
 C   -2.566800   -0.766400    0.350200
 C   -2.704400    0.406800   -0.447200
 C   -3.971200    0.789700   -0.885100
 C   -1.220000   -1.196500    0.920600
 C   -0.320700   -0.001200    0.824400
 C   -0.290900    0.374400   -0.643500
 C   -1.498300    1.236000   -0.876600
 O   -0.989600   -2.311300    1.329200
 O   -1.575500    2.364400   -1.302000
 C    0.998500    0.386100    0.182000
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C	1.479500	1.753400	0.645100
C	2.037000	-0.640600	-0.179000
C	2.626000	-0.645800	-1.447400
C	3.601300	-1.586300	-1.767200
C	3.999200	-2.531600	-0.821600
C	3.412900	-2.533800	0.442400
C	2.435100	-1.593200	0.762200
O	0.769300	2.575600	1.176700
O	2.771700	1.942000	0.376900
C	3.319900	3.228800	0.746600
H	4.366900	3.186200	0.459700
H	3.219600	3.384700	1.820500
H	2.804200	4.025000	0.209800
H	2.319800	0.088500	-2.184300
H	4.049300	-1.582500	-2.754400
H	4.757000	-3.265300	-1.071700
H	3.710400	-3.271100	1.179300
H	1.967800	-1.606700	1.739700
H	-0.706100	0.818800	1.425000
H	-0.321400	-0.502600	-1.286600
H	-6.070700	0.332300	-0.916000
H	-4.062900	1.684200	-1.489800
H	-5.826000	-1.728400	0.441300
H	-3.578100	-2.415800	1.256300

For D(X=Me)

NQ(Naphthaquinone)

C	-2.675400	0.698100	0.000000
C	-2.675400	-0.698000	0.000000
C	-1.471600	1.396500	0.000000
C	-0.260000	0.703700	0.000000
C	-0.260100	-0.703700	0.000000
C	-1.471600	-1.396400	0.000000
C	1.024300	1.460300	0.000000
C	2.278400	0.669700	0.000000
C	2.278300	-0.669800	0.000000
C	1.024200	-1.460400	0.000100
O	1.062100	2.681800	0.000000
O	1.062000	-2.681900	0.000000
H	-1.452500	2.479100	0.000000
H	-1.452700	-2.479100	0.000000
H	3.196700	-1.246100	0.000000
H	3.196800	1.246000	0.000000
H	-3.613600	1.240200	0.000000
H	-3.613700	-1.240100	0.000000

CH_3 carbene

C	-2.694100	-0.849000	0.312500
C	-1.783000	-0.264000	-0.662100
C	-0.605800	0.398600	-0.167400
O	-0.685400	1.588700	0.118300
O	0.504600	-0.339900	-0.157200
C	1.764800	0.338400	0.151000
C	2.871100	-0.685800	0.026500
H	1.696200	0.745900	1.160600
H	1.887600	1.163600	-0.552100
H	2.723600	-1.510700	0.726900
H	3.828200	-0.210000	0.254700
H	2.921400	-1.088700	-0.987200
H	-3.452200	-1.500700	-0.122500

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 H   -3.234800    0.060400    0.652500
 H   -2.241200   -1.279000    1.215200
EPINT
 C    1.177500    0.421200    0.002300
 C    2.576800    0.193400   -0.000800
 C    0.290200   -0.720300   -0.006800
 C    0.804500   -2.040100   -0.024700
 C    2.152300   -2.261600   -0.029800
 C    3.123700   -1.183000   -0.015500
 O    4.345800   -1.405400   -0.016400
 H    0.136900   -2.886600   -0.039500
 H    2.539600   -3.273300   -0.046100
 C   -3.321900   -0.148900    0.003100
 O   -4.463300   -0.579900    0.019400
 O   -3.013800    1.158400   -0.029100
 C   -4.130400    2.073700   -0.045700
 H   -4.733600    1.951600    0.854200
 H   -4.747000    1.902500   -0.928300
 O   -1.004400   -0.397400   -0.003100
 C   -2.146600   -1.031100    0.015900
 C    3.454300    1.288900    0.010000
 H    4.518800    1.089900    0.007500
 C    2.970400    2.586000    0.023700
 C    1.585000    2.811600    0.026900
 H    1.203100    3.826100    0.037700
 C    0.698700    1.748700    0.016800
 H   -0.368800    1.927700    0.019900
 H    3.656900    3.424600    0.032200
 C   -2.300000   -2.502400    0.054300
 H   -1.877500   -2.976500   -0.839500
 H   -1.802200   -2.933800    0.930700
 H   -3.360100   -2.740400    0.102100
 C   -3.502000    3.479000   -0.089000
 H   -2.897600    3.626400    0.781600
 H   -2.894200    3.571100   -0.964800
 H   -4.277400    4.215800   -0.113900
EPTS2
 C    1.558700   -1.992600   -0.901500
 C    2.881500   -1.865400   -0.589100
 C    0.652900   -0.932100   -0.687300
 C    1.117000    0.381200   -0.296100
 C    2.491900    0.519600    0.037700
 C    3.420000   -0.630700   -0.036300
 O    4.608300   -0.545700    0.311800
 H    1.165000   -2.923400   -1.294200
 H    3.573400   -2.685900   -0.737000
 C   -2.373800   -0.381300    0.586700
 O   -2.942500   -0.404900    1.665100
 O   -2.763100    0.342000   -0.472000
 C   -3.991500    1.119600   -0.344200
 H   -4.048100    1.511800    0.670900
 H   -3.853200    1.941600   -1.045100
 O   -0.694500   -1.195500   -0.954900
 C   -1.175700   -1.199200    0.318400
 C    3.001200    1.784800    0.378400
 C    2.190200    2.903900    0.367100
 C    0.841600    2.776800   -0.007600
 C    0.312600    1.543100   -0.332600
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H	-0.724400	1.466700	-0.628700
H	4.051600	1.858200	0.631600
H	2.593500	3.875500	0.626800
H	0.207600	3.655200	-0.048500
C	-0.741500	-2.181000	1.351800
H	-0.126100	-2.963200	0.908500
H	-0.165800	-1.718900	2.161800
H	-1.630500	-2.620100	1.813300
C	-5.208900	0.283600	-0.696400
H	-5.339800	-0.541600	0.005900
H	-6.100700	0.914400	-0.651600
H	-5.125300	-0.119400	-1.708100

EP prod

C	-4.286200	-1.081300	0.157200
C	-3.405500	-2.064900	-0.297300
C	-3.828700	0.216900	0.340800
C	-2.488600	0.539000	0.095300
C	-1.586300	-0.467100	-0.304500
C	-2.065600	-1.761200	-0.524700
C	-2.062500	1.965600	0.148200
C	-0.757900	2.281300	-0.458000
C	0.111600	1.321500	-0.799800
C	-0.151400	-0.107900	-0.511800
O	-2.780000	2.847500	0.611100
O	0.669700	-1.064500	-1.208800
C	0.972500	-0.880900	0.166200
C	2.259500	-0.127100	0.486100
C	0.740900	-2.025600	1.125300
O	2.518900	0.241000	1.610200
O	3.036600	0.050600	-0.580500
C	4.308800	0.747100	-0.388200
H	-0.241100	-2.473900	1.002600
H	0.841700	-1.666100	2.149600
H	1.499400	-2.795500	0.955600
H	-5.326100	-1.323700	0.341500
H	-3.763500	-3.071400	-0.480400
H	-4.501300	1.006600	0.652100
H	-1.394300	-2.523600	-0.896600
H	-0.530900	3.330900	-0.603800
H	1.070700	1.564800	-1.241500
C	5.410500	-0.222800	-0.004200
H	4.167500	1.522500	0.364100
H	4.498900	1.209200	-1.355800
H	5.214100	-0.683200	0.965800
H	6.357300	0.319900	0.061900
H	5.518900	-1.007700	-0.755800

AQ

For A(X=H)

AQ(Anthraquinone)

C	-2.810300	1.404800	0.000000
C	-3.995600	0.707200	0.000000
C	-1.570400	0.716800	0.000000
C	-1.570400	-0.716800	0.000000
C	-2.810300	-1.404800	0.000000
C	-3.995600	-0.707200	0.000000
C	-0.330100	1.400300	0.000000

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 C    0.863600    0.714500    0.000000
 C    0.863600   -0.714500    0.000000
 C   -0.330100   -1.400300    0.000000
 C    2.146300    1.468000    0.000000
 C    3.395400    0.670300    0.000000
 C    3.395400   -0.670300    0.000000
 C    2.146300   -1.468000    0.000000
 O    2.193500    2.690600    0.000000
 O    2.193500   -2.690600    0.000000
 H   -2.808700    2.489100    0.000000
 H   -4.938400    1.241600    0.000000
 H   -4.938400   -1.241600    0.000000
 H   -2.808700   -2.489100    0.000000
 H   -0.311300    2.484100    0.000000
 H   -0.311300   -2.484100    0.000000
 H    4.316500   -1.242500    0.000000
 H    4.316500    1.242500    0.000000
H carbene
 C   -1.825500   -0.799000    0.000000
 H   -2.629300   -0.040900   -0.000100
 C   -0.568500    0.054400    0.000000
 O   -0.529400    1.270100    0.000000
 O    0.521900   -0.723300    0.000000
 C    1.791700   -0.037400    0.000000
 H    2.546200   -0.818600    0.000000
 H    1.878400    0.588500    0.889500
 H    1.878400    0.588500   -0.889500
EPINT
 C    0.375700    0.071700    0.311200
 C    1.011400    1.346900    0.128200
 C   -1.052500    0.047000    0.534600
 C   -1.801900    1.248700    0.634300
 C   -1.201700    2.460900    0.491000
 C    0.220900    2.602300    0.193900
 O    0.735400    3.714700    0.035400
 H   -2.850300    1.192900    0.886000
 H   -1.766000    3.375700    0.625900
 C   -3.981000   -1.221700    0.078300
 O   -5.039300   -1.831400    0.185600
 O   -3.810200   -0.171900   -0.753800
 C   -4.942800    0.191100   -1.571700
 H   -5.790500    0.466900   -0.944100
 H   -5.222000   -0.637900   -2.222300
 H   -4.610100    1.042500   -2.160100
 O   -1.566800   -1.153900    0.749100
 C   -2.796600   -1.654700    0.776100
 H   -2.818200   -2.634600    1.227000
 C    2.370500    1.406000   -0.104800
 C    3.164200    0.239800   -0.165700
 C    4.564700    0.288900   -0.398200
 C    5.305200   -0.867900   -0.453800
 H    6.373300   -0.821800   -0.631300
 C    2.530400   -1.034900    0.010100
 C    1.139100   -1.086500    0.236100
 C    4.679600   -2.128300   -0.281500
 H    5.277500   -3.031100   -0.329400
 C    3.326600   -2.211800   -0.056500
 H    2.848900   -3.176500    0.074500
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 H    2.831000    2.377600   -0.242200
 H    5.039900    1.254500   -0.531500
 H    0.663100   -2.052800    0.349100
EPTS
 C    0.599900    3.128900   -0.574000
 C   -0.621400    3.653200   -0.276400
 C    0.853000    1.739900   -0.466900
 C   -0.219500    0.797700   -0.217400
 C   -1.517500    1.342000    0.085000
 C   -1.740100    2.807300    0.136900
 O   -2.820100    3.303800    0.474400
 H    1.429600    3.767600   -0.855200
 H   -0.801300    4.720400   -0.322500
 C    3.302300   -0.335700    0.635900
 O    3.811200   -0.689600    1.693000
 O    3.386300   -1.036300   -0.515400
 C    4.185000   -2.237100   -0.475700
 H    5.218700   -1.996200   -0.225100
 H    4.123700   -2.657200   -1.476300
 H    3.783600   -2.935700    0.259000
 O    2.153300    1.352200   -0.713300
 C    2.566700    0.893500    0.502100
 H    2.419500    1.532400    1.360000
 C   -2.595800    0.494700    0.260800
 C   -2.471600   -0.902300    0.126800
 C   -1.188200   -1.445700   -0.216900
 C   -0.092500   -0.579100   -0.377600
 C   -3.572200   -1.784100    0.300500
 C   -1.061300   -2.855600   -0.377500
 C   -3.413400   -3.139500    0.140800
 H   -4.257600   -3.805600    0.275500
 C   -2.146300   -3.678300   -0.202800
 H   -2.039300   -4.749900   -0.326100
 H   -0.093100   -3.268800   -0.638000
 H    0.870200   -1.009100   -0.625900
 H   -3.562900    0.930800    0.483400
 H   -4.539700   -1.368800    0.560400
EP prod
 C   -4.652100   -2.031600   -0.030600
 C   -5.240100   -0.788900    0.313300
 C   -3.300200   -2.125800   -0.262700
 C   -2.468900   -0.979100   -0.159800
 C   -3.063400    0.277700    0.183900
 C   -4.464400    0.340200    0.417300
 C   -1.071200   -1.040300   -0.384900
 C   -0.279900    0.081400   -0.284500
 C   -0.877100    1.341000    0.026600
 C   -2.235700    1.418700    0.263000
 C    1.199800    0.010900   -0.490400
 C    1.908900    1.292800   -0.682700
 C    1.333000    2.473200   -0.419800
 C   -0.063400    2.587200    0.035700
 O    1.684400   -1.094200   -1.285600
 O   -0.530200    3.673200    0.368000
 C    1.955800   -1.153000    0.100000
 C    3.370400   -1.063300    0.607100
 O    3.629800   -1.241800    1.776400
 O    4.261200   -0.782300   -0.341700
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C	5.644400	-0.677900	0.079000
H	6.202200	-0.459900	-0.827400
H	5.972300	-1.620000	0.516900
H	5.754300	0.127900	0.804200
H	-6.307600	-0.734400	0.492400
H	-5.277700	-2.913200	-0.110500
H	-4.909800	1.294300	0.676900
H	-2.669300	2.383800	0.498300
H	-0.629700	-1.993700	-0.652100
H	1.879800	3.402600	-0.529300
H	2.936700	1.233100	-1.019700
H	-2.852300	-3.077800	-0.525600
H	1.364600	-1.862000	0.673300

For B(X=CO2Me)

AQ(Anthraquinone)

C	-2.810300	1.404800	0.000000
C	-3.995600	0.707200	0.000000
C	-1.570400	0.716800	0.000000
C	-1.570400	-0.716800	0.000000
C	-2.810300	-1.404800	0.000000
C	-3.995600	-0.707200	0.000000
C	-0.330100	1.400300	0.000000
C	0.863600	0.714500	0.000000
C	0.863600	-0.714500	0.000000
C	-0.330100	-1.400300	0.000000
C	2.146300	1.468000	0.000000
C	3.395400	0.670300	0.000000
C	3.395400	-0.670300	0.000000
C	2.146300	-1.468000	0.000000
O	2.193500	2.690600	0.000000
O	2.193500	-2.690600	0.000000
H	-2.808700	2.489100	0.000000
H	-4.938400	1.241600	0.000000
H	-4.938400	-1.241600	0.000000
H	-2.808700	-2.489100	0.000000
H	-0.311300	2.484100	0.000000
H	-0.311300	-2.484100	0.000000
H	4.316500	-1.242500	0.000000
H	4.316500	1.242500	0.000000

CO_2Me carbene

C	-1.255300	-0.333900	0.211100
C	0.000400	-0.374700	0.906100
C	1.255100	-0.337300	0.207200
O	-1.640100	-1.391000	-0.264800
O	1.640600	-1.390000	-0.276500
O	-1.898000	0.821600	0.230500
O	1.897700	0.818900	0.234200
C	-3.227700	0.846600	-0.364800
C	3.227300	0.848600	-0.360700
H	3.581000	1.862300	-0.198600
H	3.163100	0.627700	-1.425000
H	3.873100	0.128500	0.139600
H	-3.582300	1.860900	-0.208600
H	-3.872900	0.128800	0.139400
H	-3.162800	0.619800	-1.427800

EPINT

C	-1.030800	0.244900	-0.310200
C	-1.983900	1.291000	-0.552700

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 C    0.371000    0.537100   -0.473400
 C    0.811600    1.823700   -0.929500
 C   -0.077300    2.807900   -1.185200
 C   -1.526700    2.637800   -0.976600
 O   -2.300700    3.569200   -1.181400
 H    1.867400    1.960100   -1.126000
 H    0.243400    3.759500   -1.592100
 C    3.081700    0.633700    0.905600
 O    4.257900    0.821900    1.169700
 O    2.080600    1.301600    1.549500
 C    2.487200    2.250300    2.553400
 H    3.145900    3.005700    2.123900
 H    2.998500    1.744500    3.373200
 H    1.566100    2.707600    2.907500
 O    1.201500   -0.445300   -0.255200
 C    2.568400   -0.318800   -0.056500
 C   -3.326500    1.040000   -0.387700
 C   -3.797300   -0.234400    0.015300
 C   -5.176900   -0.507600    0.180800
 C   -5.597600   -1.758200    0.577400
 H   -6.655200   -1.959200    0.700900
 C   -2.845500   -1.276700    0.267800
 C   -1.469800   -1.003800    0.108100
 C   -4.659600   -2.786800    0.827000
 H   -5.009200   -3.764100    1.138500
 C   -3.311800   -2.553300    0.677700
 H   -2.591200   -3.340300    0.868900
 H   -4.034600    1.839500   -0.572400
 H   -5.896400    0.280700   -0.009000
 H   -0.748200   -1.782800    0.320300
 C    3.258900   -1.455700   -0.631800
 O    4.575900   -1.505600   -0.343600
 C    5.304600   -2.605600   -0.919700
 H    6.336300   -2.458200   -0.608700
 H    4.927600   -3.557300   -0.543200
 H    5.229600   -2.590400   -2.007700
 O    2.702300   -2.296800   -1.328000

EPTS
 C   -1.225200   -2.172800   -1.508900
 C   -0.571000   -3.267300   -1.059300
 C   -0.784100   -0.851000   -1.167400
 C    0.528300   -0.649300   -0.593700
 C    1.232700   -1.803900   -0.100700
 C    0.645300   -3.159500   -0.232800
 O    1.151600   -4.160600    0.266400
 H   -2.139000   -2.250100   -2.081500
 H   -0.929100   -4.267800   -1.271100
 C   -1.892300    2.051800   -0.050900
 O   -2.329300    2.676100    0.900800
 O   -1.188500    2.655700   -1.049100
 C   -1.042100    4.084600   -0.938500
 H   -2.018300    4.570400   -0.954500
 H   -0.457100    4.382300   -1.805700
 H   -0.521300    4.347200   -0.017000
 O   -1.605600    0.158600   -1.557400
 C   -2.059200    0.629700   -0.305300
 C    2.500000   -1.667100    0.417900
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 C    3.156500   -0.412500    0.451200
 C    2.482000    0.728400   -0.093600
 C    1.175400    0.580700   -0.604300
 C    4.461400   -0.257300    0.976700
 C    3.145800    1.984100   -0.096900
 C    5.075900    0.976400    0.964200
 H    6.074900    1.087500    1.369200
 C    4.414600    2.103000    0.422500
 H    4.914000    3.064600    0.418900
 H    2.636900    2.847300   -0.510400
 H    0.668600    1.447300   -1.007600
 H    3.012100   -2.550500    0.781400
 H    4.970700   -1.121800    1.387200
 C   -3.001000   -0.242100    0.393700
 O   -3.462700   -1.276700   -0.070700
 O   -3.329500    0.208600    1.619600
 C   -4.315500   -0.561900    2.334300
 H   -4.451300   -0.042900    3.280100
 H   -5.254100   -0.592800    1.780000
 H   -3.959000   -1.578400    2.504800
EP prod
 C   -4.811100   -1.857800   -0.552100
 C   -5.435100   -0.719300    0.014100
 C   -3.461600   -1.857100   -0.817500
 C   -2.671400   -0.715500   -0.524200
 C   -3.302200    0.436700    0.044500
 C   -4.698700    0.404100    0.304400
 C   -1.275700   -0.685300   -0.774900
 C   -0.520700    0.426900   -0.478800
 C   -1.158800    1.594800    0.045800
 C   -2.513900    1.579500    0.306300
 C    0.958800    0.457400   -0.709600
 C    1.578100    1.800500   -0.798800
 C    0.962300    2.897900   -0.342000
 C   -0.398700    2.861300    0.224300
 O    1.482600   -0.547900   -1.592400
 O   -0.882100    3.849300    0.767700
 C    1.846900   -0.692200   -0.240000
 C    1.264600   -1.931700    0.463800
 C    3.319400   -0.504100    0.106100
 O    3.753200   -0.752800    1.208200
 O    4.037200   -0.076100   -0.922900
 C    5.459300    0.104500   -0.689200
 H    5.860100    0.444600   -1.639600
 H    5.907700   -0.843600   -0.395600
 H    5.616200    0.850700    0.088800
 H   -6.499800   -0.738600    0.215500
 H   -5.406100   -2.735700   -0.776200
 H   -5.172900    1.279700    0.734000
 H   -2.979000    2.476200    0.699300
 H   -0.809900   -1.556500   -1.218200
 H    1.448100    3.866500   -0.366700
 H    2.577100    1.848400   -1.213300
 H   -2.984800   -2.729800   -1.249600
 O    0.876500   -1.861200    1.734300
 O    1.195300   -2.974600   -0.138300
 C    0.880100   -0.631600    2.505600
 H    1.860800   -0.163600    2.477000
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H	0.101400	0.037800	2.143600
H	0.649900	-0.944100	3.520700

For C(X=Ph)

AQ(Anthraquinone)

C	-2.810300	1.404800	0.000000
C	-3.995600	0.707200	0.000000
C	-1.570400	0.716800	0.000000
C	-1.570400	-0.716800	0.000000
C	-2.810300	-1.404800	0.000000
C	-3.995600	-0.707200	0.000000
C	-0.330100	1.400300	0.000000
C	0.863600	0.714500	0.000000
C	0.863600	-0.714500	0.000000
C	-0.330100	-1.400300	0.000000
C	2.146300	1.468000	0.000000
C	3.395400	0.670300	0.000000
C	3.395400	-0.670300	0.000000
C	2.146300	-1.468000	0.000000
O	2.193500	2.690600	0.000000
O	2.193500	-2.690600	0.000000
H	-2.808700	2.489100	0.000000
H	-4.938400	1.241600	0.000000
H	-4.938400	-1.241600	0.000000
H	-2.808700	-2.489100	0.000000
H	-0.311300	2.484100	0.000000
H	-0.311300	-2.484100	0.000000
H	4.316500	-1.242500	0.000000
H	4.316500	1.242500	0.000000

Ph carbene

C	0.538000	-1.109100	0.003900
C	1.745600	-0.387500	0.282800
C	-0.722700	-0.471000	-0.000400
C	-0.905000	0.931200	0.187500
C	-1.876600	-1.274100	-0.221400
C	-2.169000	1.489400	0.153200
C	-3.283000	0.668900	-0.071600
C	-3.140400	-0.709400	-0.260000
O	2.169300	-0.289900	1.431400
O	2.410700	0.042000	-0.807300
C	3.737000	0.577700	-0.589900
H	4.107700	0.831200	-1.580000
H	4.377300	-0.171800	-0.124200
H	3.692800	1.467400	0.038200
H	-1.734300	-2.338800	-0.360000
H	-4.272400	1.111700	-0.099100
H	-4.014000	-1.326200	-0.431400
H	-0.038800	1.558700	0.361900
H	-2.303200	2.554700	0.296800

CHTS1/CPTS1

C	0.039700	-2.156600	-0.483900
C	1.211300	-2.026100	0.423400
C	1.112300	-1.417800	1.638300
C	-0.081600	-0.675800	2.051400
O	0.086800	-2.899300	-1.454900
O	-0.121100	-0.102600	3.140300
H	2.058900	-2.653400	0.185600
C	2.408700	-0.242200	-0.558200
C	3.768400	-0.558100	-0.147400

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 O    4.633400    0.002900   -1.032100
 O    4.122200   -1.306100    0.749900
 C    6.009500   -0.431100   -0.950000
 H    6.077800   -1.510000   -1.092800
 H    6.521900    0.091700   -1.753900
 H    6.437600   -0.160200    0.015300
 H    1.941200   -1.434500    2.334900
 C   -1.231700   -0.651500    1.104200
 C   -1.174800   -1.376900   -0.127600
 C   -2.253300   -1.361200   -0.985900
 C   -2.365100    0.065000    1.422100
 C   -3.480200    0.105200    0.550200
 C   -3.423300   -0.624900   -0.681800
 C   -4.651800    0.844300    0.858700
 C   -4.539300   -0.587500   -1.557700
 C   -5.659900    0.140000   -1.229500
 H   -6.508100    0.163400   -1.903700
 C   -5.716400    0.861000   -0.012600
 H   -6.607200    1.428400    0.230600
 H   -4.495300   -1.141700   -2.488700
 H   -4.694700    1.395500    1.791400
 H   -2.398000    0.606500    2.360500
 H   -2.196400   -1.921200   -1.912300
 C    1.873300    1.072000   -0.433900
 C    0.718100    1.406400   -1.188400
 C    2.482400    2.091100    0.349200
 C    0.209100    2.695400   -1.175200
 H    0.259100    0.638600   -1.797700
 C    1.962600    3.373300    0.369400
 H    3.359600    1.852900    0.939200
 C    0.828300    3.675000   -0.394300
 H   -0.662700    2.944600   -1.767800
 H    2.430300    4.143100    0.971300
 H    0.427200    4.682200   -0.380400
CHINT
 C    1.448200    0.441900    0.064300
 C    1.759900   -0.711500    0.850400
 C    0.078300    0.997600   -0.005100
 C   -0.586200   -0.860000    1.650200
 C    0.720900   -1.389300    1.684100
 O   -0.214000    1.943600   -0.708700
 O    1.028600   -2.376400    2.397800
 H   -1.330000   -1.359500    2.260300
 C   -2.354000    0.366500    0.257600
 C   -2.908700    1.744100    0.084300
 C   -3.093000   -0.758700   -0.214800
 O   -3.511600    2.133800   -0.894600
 O   -2.640700    2.528100    1.145400
 C   -3.035500    3.914700    1.035400
 H   -4.113700    3.987300    0.893100
 H   -2.518900    4.382900    0.197800
 H   -2.740900    4.372300    1.976000
 C   -4.401900   -0.604200   -0.769200
 C   -2.530500   -2.069100   -0.253200
 C   -5.045900   -1.660300   -1.385400
 C   -4.426300   -2.910500   -1.484000
 C   -3.160600   -3.102500   -0.921300
 H   -4.886000    0.359200   -0.738700
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H   -6.037100   -1.513200   -1.797200
H   -4.940600   -3.737200   -1.959700
H   -2.692400   -4.078700   -0.958400
H   -1.599400   -2.269900    0.258400
C   -1.007200    0.333000    0.907200
H   -1.134500    1.120500    1.683200
C    2.438700    1.070000   -0.669700
H    2.183300    1.943400   -1.258000
C    3.052200   -1.190900    0.855700
H    3.276000   -2.063100    1.458400
C    4.080300   -0.570600    0.105900
C    5.413700   -1.058400    0.101000
H    5.653400   -1.935900    0.691300
C    6.385700   -0.428200   -0.640400
H    7.400800   -0.808400   -0.637000
C    3.766500    0.589900   -0.674200
C    4.793600    1.216800   -1.429800
C    6.074400    0.718500   -1.412300
H    6.854200    1.201700   -1.989400
H    4.550500    2.093900   -2.019500

CHTS2
C   -1.674100    0.195000   -0.173000
C   -1.944100   -1.179000    0.097700
C   -0.285700    0.666300   -0.344600
C    0.839500   -0.253600    0.191400
C    0.510000   -1.649800    0.229600
C   -0.819700   -2.155500    0.233000
O   -0.008100    1.704500   -0.910500
O   -1.061000   -3.373000    0.371500
H    1.080300    0.036300    1.305800
H    1.289100   -2.382200    0.392900
C    2.200900    0.303900    0.155000
C    2.313000    1.771500    0.450800
C    3.414300   -0.480600    0.037200
O    1.744800    2.329600    1.366900
O    3.144400    2.372900   -0.403400
C    3.339300    3.795100   -0.218700
H    4.046600    4.088300   -0.989600
H    3.744700    3.993000    0.773500
H    2.392700    4.320000   -0.344500
C    3.465100   -1.616300   -0.800700
C    4.598600   -0.081700    0.698200
C    4.656900   -2.301000   -0.991700
C    5.813600   -1.899300   -0.320200
C    5.778700   -0.789800    0.528100
H    2.576200   -1.940900   -1.325700
H    4.683800   -3.155300   -1.657600
H    6.737300   -2.450000   -0.454800
H    6.673900   -0.478300    1.052800
H    4.585500    0.781000    1.353300
C   -4.056400    0.687500   -0.173400
C   -4.331600   -0.692900    0.094700
C   -3.248400   -1.599600    0.217300
C   -5.681900   -1.108800    0.225100
H   -5.892100   -2.153400    0.426500
H   -3.442300   -2.648700    0.407200
C   -5.138700    1.598100   -0.298100
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 H   -4.925800    2.641900   -0.500800
 C   -2.709500    1.097700   -0.312400
 H   -2.484200    2.136400   -0.524600
 C   -6.709000   -0.201700    0.098400
 H   -7.737000   -0.529900    0.200400
 C   -6.436300    1.162200   -0.165300
 H   -7.257700    1.862700   -0.262000

CHprod
 C    0.639200   -1.361500   -0.139100
 C    0.837200   -0.079700    0.210300
 C   -0.698500   -1.959100   -0.345900
 C   -1.878400   -1.080800   -0.144400
 C   -1.693700    0.281100    0.238100
 C   -0.329400    0.830300    0.440900
 C   -3.148600   -1.579500   -0.324200
 C   -4.289900   -0.762300   -0.136700
 C   -4.105200    0.606600    0.245900
 C   -2.788700    1.095900    0.425200
 C   -5.607400   -1.255500   -0.314800
 C   -6.692300   -0.432200   -0.123200
 C   -6.510300    0.919100    0.254100
 C   -5.245700    1.428500    0.434600
 C    2.198600    0.543900    0.464600
 C    3.375900   -0.417100    0.353300
 C    2.413600    1.743500   -0.464200
 C    3.858000   -0.843600   -0.889900
 C    3.986700   -0.896600    1.515800
 C    5.056100   -1.787100    1.440700
 C    5.530200   -2.207000    0.199400
 C    4.928800   -1.731800   -0.965200
 O    2.049800    1.798900   -1.615400
 O    3.114200    2.702900    0.151600
 C    3.434000    3.867300   -0.641800
 H    4.004100    4.517200    0.016700
 H    2.518900    4.360600   -0.969900
 H    4.028600    3.582400   -1.510000
 H    5.519100   -2.149100    2.351600
 H    3.623400   -0.571600    2.484900
 H    3.396500   -0.477600   -1.799900
 H    5.293000   -2.051600   -1.934900
 H    6.363500   -2.897600    0.139500
 H    2.182300    0.947100    1.479600
 O   -0.138400    1.986200    0.793900
 O   -0.800200   -3.134900   -0.670600
 H   -5.104200    2.463800    0.723900
 H   -7.376500    1.553500    0.400600
 H   -5.745200   -2.291200   -0.604300
 H   -7.696000   -0.816900   -0.261400
 H   -3.268500   -2.616900   -0.614200
 H   -2.632500    2.128100    0.715900
 H    1.468600   -2.041100   -0.294100
CP prod
 C   -6.537000    0.257700    0.527100
 C   -6.464800   -0.969500   -0.173400
 C   -5.392000    0.964200    0.816200
 C   -4.123200    0.473300    0.415200
 C   -4.050100   -0.769200   -0.292000
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C	-5.248700	-1.472300	-0.575700
C	-2.921800	1.171500	0.700900
C	-1.695400	0.684700	0.313300
C	-1.622500	-0.567100	-0.414900
C	-2.779500	-1.256200	-0.693000
C	-0.440200	1.443800	0.712000
C	0.699100	0.479900	0.571300
C	0.677100	0.025500	-0.877700
C	-0.297700	-1.112000	-0.924000
O	-0.424400	2.609300	1.044300
O	-0.120300	-2.264300	-1.255900
C	2.002600	0.349200	-0.217200
C	2.611900	1.649000	-0.724900
O	2.053000	2.420100	-1.472400
O	3.829300	1.846500	-0.218300
C	4.493700	3.077700	-0.590600
H	3.908500	3.934700	-0.258100
H	4.629800	3.117500	-1.671100
H	5.454200	3.047600	-0.083300
H	-7.502800	0.640300	0.836100
H	-5.446100	1.904500	1.353600
H	-7.376100	-1.513800	-0.392500
H	-5.191700	-2.412300	-1.113200
H	-2.966900	2.103500	1.253800
H	-2.716900	-2.186700	-1.246800
H	0.579800	-0.355200	1.258400
H	0.366000	0.831100	-1.538700
C	2.955600	-0.730800	0.220500
C	3.494400	-1.600200	-0.733400
C	3.333200	-0.866600	1.559000
C	4.400200	-2.588500	-0.353800
H	3.198200	-1.507300	-1.772300
C	4.237200	-1.857200	1.939400
H	2.922800	-0.195000	2.304900
C	4.773900	-2.719500	0.983800
H	4.807800	-3.259700	-1.101200
H	4.521000	-1.954900	2.981100
H	5.475000	-3.491500	1.279800

For D(X=Me)

AQ(Anthraquinone)

C	-2.810300	1.404800	0.000000
C	-3.995600	0.707200	0.000000
C	-1.570400	0.716800	0.000000
C	-1.570400	-0.716800	0.000000
C	-2.810300	-1.404800	0.000000
C	-3.995600	-0.707200	0.000000
C	-0.330100	1.400300	0.000000
C	0.863600	0.714500	0.000000
C	0.863600	-0.714500	0.000000
C	-0.330100	-1.400300	0.000000
C	2.146300	1.468000	0.000000
C	3.395400	0.670300	0.000000
C	3.395400	-0.670300	0.000000
C	2.146300	-1.468000	0.000000
O	2.193500	2.690600	0.000000
O	2.193500	-2.690600	0.000000
H	-2.808700	2.489100	0.000000
H	-4.938400	1.241600	0.000000

H	-4.938400	-1.241600	0.000000
H	-2.808700	-2.489100	0.000000
H	-0.311300	2.484100	0.000000
H	-0.311300	-2.484100	0.000000
H	4.316500	-1.242500	0.000000
H	4.316500	1.242500	0.000000

CH_3 carbene

C	-2.694100	-0.849000	0.312500
C	-1.783000	-0.264000	-0.662100
C	-0.605800	0.398600	-0.167400
O	-0.685400	1.588700	0.118300
O	0.504600	-0.339900	-0.157200
C	1.764800	0.338400	0.151000
C	2.871100	-0.685800	0.026500
H	1.696200	0.745900	1.160600
H	1.887600	1.163600	-0.552100
H	2.723600	-1.510700	0.726900
H	3.828200	-0.210000	0.254700
H	2.921400	-1.088700	-0.987200
H	-3.452200	-1.500700	-0.122500
H	-3.234800	0.060400	0.652500
H	-2.241200	-1.279000	1.215200

EPINT

C	-0.726700	0.055600	-0.431600
C	-1.330400	1.360200	-0.381400
C	0.675700	-0.023100	-0.738100
C	1.428600	1.127300	-1.050400
C	0.861000	2.368900	-1.031900
C	-0.528900	2.579900	-0.661700
O	-1.026000	3.715400	-0.619800
H	2.455700	1.006400	-1.370800
H	1.426600	3.239800	-1.340400
C	3.461800	-1.043200	0.146700
O	4.608600	-1.470700	0.180300
O	2.997400	-0.068500	0.952100
C	3.909000	0.479500	1.948100
H	4.536000	-0.326300	2.328800
H	3.247200	0.826800	2.740600
O	1.189900	-1.260000	-0.816200
C	2.448300	-1.669300	-0.697200
C	-2.670800	1.478300	-0.071300
C	-3.474400	0.349400	0.196600
C	-4.856400	0.460800	0.508700
C	-5.608500	-0.659600	0.768200
H	-6.661900	-0.565100	1.005100
C	-2.871100	-0.952500	0.156900
C	-1.499100	-1.065600	-0.145000
C	-5.013200	-1.946600	0.729900
H	-5.619800	-2.820600	0.937900
C	-3.679800	-2.090800	0.433800
H	-3.226100	-3.075600	0.405800
H	-3.107300	2.469900	-0.035600
H	-5.308000	1.446500	0.538700
H	-1.042200	-2.047800	-0.147100
C	2.721100	-2.973900	-1.356000
H	3.144000	-2.827100	-2.359000
H	3.438500	-3.560500	-0.782800
H	1.788000	-3.529400	-1.472600

C	4.739300	1.617300	1.380500
H	5.358900	2.039100	2.176900
H	5.399600	1.268200	0.584600
H	4.098600	2.411100	0.990400

EPTS2

C	0.125600	-3.093700	-0.841700
C	1.401100	-3.495100	-0.563000
C	-0.287400	-1.756700	-0.656700
C	0.671400	-0.716300	-0.349900
C	2.016500	-1.130700	-0.041300
C	2.405400	-2.562400	-0.072300
O	3.535400	-2.948100	0.259600
H	-0.618000	-3.805900	-1.182000
H	1.702300	-4.528300	-0.687300
C	-2.852700	-0.043000	0.628100
O	-3.400900	0.183700	1.696400
O	-2.915300	0.759500	-0.448300
C	-3.743500	1.954600	-0.350000
H	-3.655100	2.355800	0.659400
H	-3.288600	2.646800	-1.057300
O	-1.637200	-1.489200	-0.882300
C	-2.067800	-1.258900	0.394900
C	2.988600	-0.179800	0.212800
C	2.712100	1.199600	0.154800
C	1.384900	1.617100	-0.198900
C	0.397100	0.646300	-0.443400
C	3.703700	2.186700	0.409200
C	1.108000	3.012300	-0.289700
C	3.400100	3.522800	0.317100
H	4.161400	4.268900	0.513300
C	2.089500	3.937900	-0.037800
H	1.867200	4.996600	-0.108000
H	0.106900	3.331100	-0.558700
H	-0.598800	0.977400	-0.708600
H	3.993300	-0.519400	0.437100
H	4.704700	1.865600	0.676200
C	-1.998800	-2.289700	1.468600
H	-1.739100	-3.263200	1.052800
H	-1.262900	-2.051400	2.245600
H	-2.970900	-2.344100	1.966600
C	-5.187500	1.656000	-0.713600
H	-5.761100	2.586700	-0.695900
H	-5.256100	1.230800	-1.717200
H	-5.640300	0.963300	-0.001900

EP prod

C	5.684200	-0.710300	-0.050400
C	5.097700	-1.945200	0.320700
C	4.898800	0.401600	-0.239000
C	3.489800	0.326900	-0.069600
C	2.896400	-0.922600	0.298600
C	3.737000	-2.049700	0.493100
C	2.651700	1.454500	-0.219300
C	1.285900	1.364400	-0.043000
C	0.685000	0.101700	0.259100
C	1.488100	-0.999200	0.452300
C	0.470300	2.610300	-0.044300
C	-0.889600	2.498900	0.510800
C	-1.464900	1.311400	0.742000

C	-0.802700	0.035000	0.381300
O	0.915500	3.689900	-0.424100
O	-1.362500	-1.158800	0.958100
C	-1.629800	-0.958800	-0.423800
C	-3.055600	-0.565200	-0.791900
C	-1.029800	-1.919000	-1.424700
H	0.030300	-2.079800	-1.248100
H	-1.166700	-1.528700	-2.433400
H	-1.545400	-2.881200	-1.355600
O	-3.354500	-0.219000	-1.913600
O	-3.907100	-0.664200	0.226100
C	-5.301700	-0.317900	-0.041900
C	-6.075500	-0.517000	1.242600
H	-5.661500	-0.962300	-0.845400
H	-5.333900	0.716600	-0.387500
H	-6.021900	-1.555000	1.577500
H	-7.125300	-0.266000	1.071500
H	-5.694400	0.129000	2.036500
H	6.758200	-0.646800	-0.181500
H	5.343400	1.350900	-0.517000
H	5.730300	-2.812900	0.468900
H	3.290100	-2.996400	0.776200
H	3.085800	2.421400	-0.446800
H	1.046100	-1.944500	0.741500
H	-1.410000	3.428400	0.710100
H	-2.468600	1.245000	1.144800

References

1. Gaussian 09, Revision A.02, M. J. Frisch et. al. Gaussian, Inc., Wallingford CT, 2016.
2. A.D. Becke, J.Chem.Phys. 98 (1993) 5648-5652
3. C. Lee, W. Yang, R.G. Parr, Phys. Rev. B 37 (1988) 785-789

4. Ditchfield, R., Hehre, W. J., Pople, J. A. Self-Consistent Molecular-Orbital Methods. IX. An Extended Gaussian-Type Basis for Molecular-Orbital Studies of Organic Molecules *J. Chem. Phys.*1971, **54**, 724-728.
5. Hariharan, P. C., Pople, J. A. The influence of polarization functions on molecular orbital hydrogenation energies, *Theor. Chim. Acta* 1973 **28**, 213-222.
6. Hehre, W. J., Ditchfield, R., Pople, J. A. Self-Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian-Type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules, *J. Chem. Phys.* 1972, **56**, 2257-2261.
7. Rassolov, Vitaly A., Pople, John A., Ratner, Mark A., Windus, Theresa L. 6-31G* basis set for atoms K through Zn, *J. Chem. Phys.* 1998, **109**, 1223-1229.
8. S. Miertus, E. Scrocco, J. Tomasi, *J. Chem. Phys.* 1981, **55**, 117– 129.
9. H. B. Schlegel, *J. Comp. Chem.*, 1982, **3**, 214-218.
10. H. B. Schlegel, *Theor. Chem. Acc.*, 1984, **66,** 333-340.
11. J. M. Bofill, *J. Comp. Chem.*, 1994, **15**, 1-11.
12. J. M. Bofill and M. Comajuan, *J. Comp. Chem.*, 1995, **16**, 1326-1338.