The capture of •H and •OH radicals by vitamin C and implications for the new source for the formation of the anion free radical

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1. Solvent effects on the geometries

As mentioned above, the single point energy calculations were performed employing the PCM model to evaluate the solvent effects on the potential energy profiles of various reactions studied herein. To validate the validity of this procedure, the effect of the solvent on geometry optimizations has been tested for the most important channel of addition reaction of •OH to C2 site. Namely, all the stationary points in this channel have been fully optimized in aqueous solution employing the PCM model. As displayed in Fig. S1, the optimized geometries in solution are close to the geometries in the gas phase overall except for the slightly different orientations of the hydroxyl group of O9-H13 for L-RC(C2-•OH). Additionally, the difference of the calculated forward and reverse barrier heights are only 1.86 and 0.29 kcal mol^{-1} based on the optimized geometries in the gas phase and in solution at the B3LYP/6-311++G** level of theory.

Therefore, it is a valid approximation to perform the single point calculation at gas phase optimized geometries in solution.

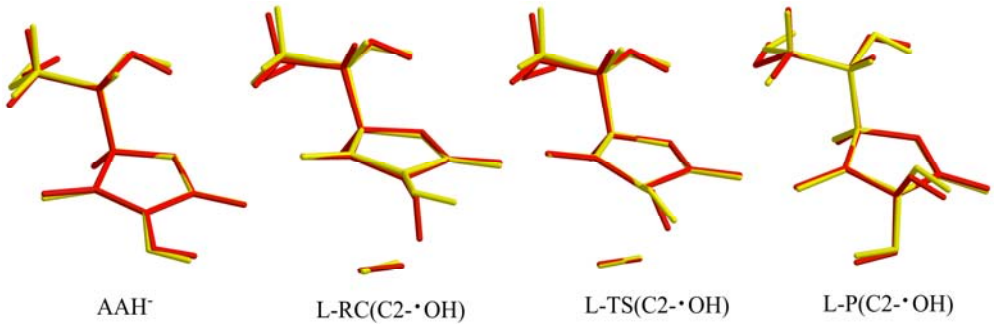
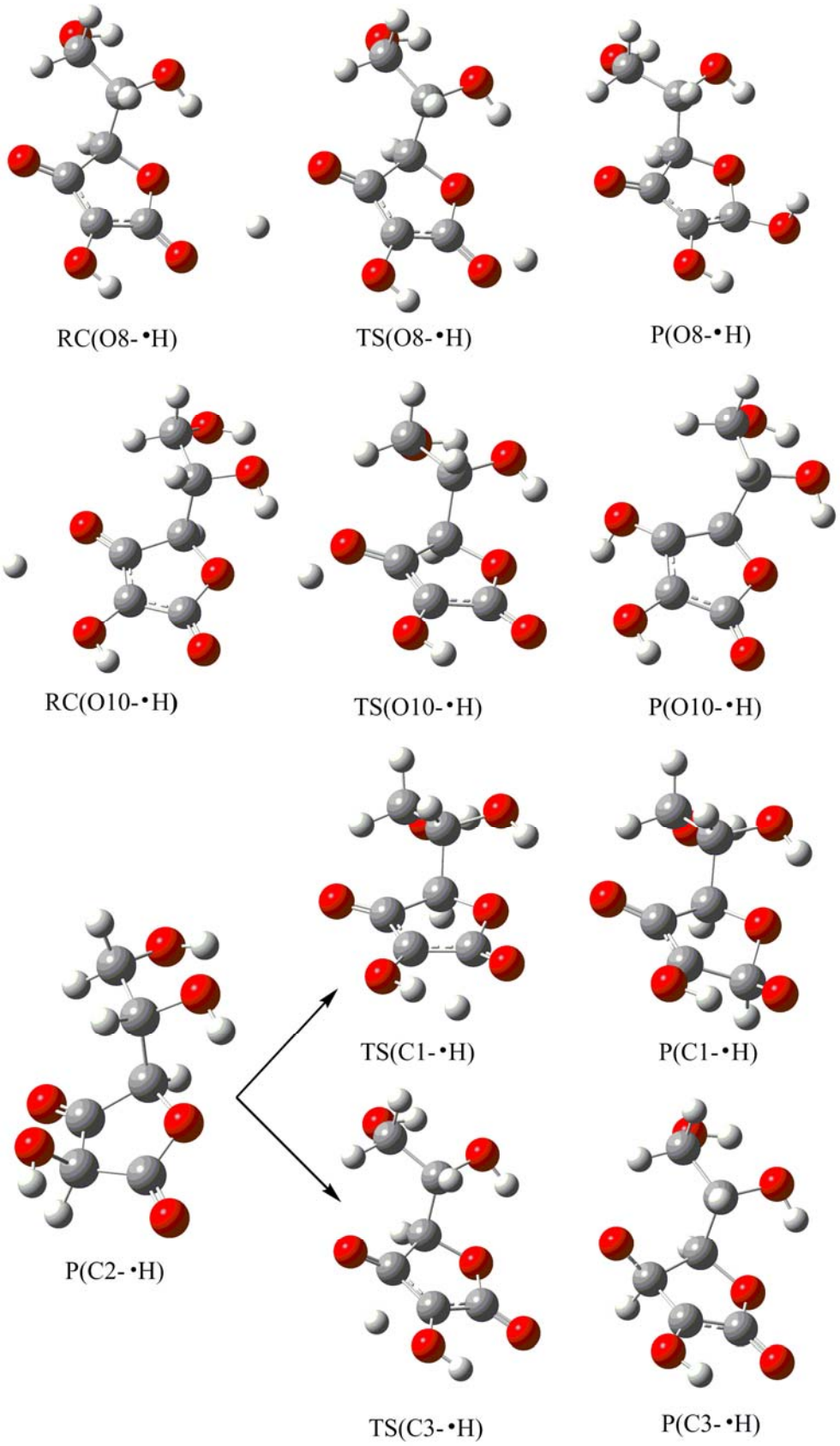
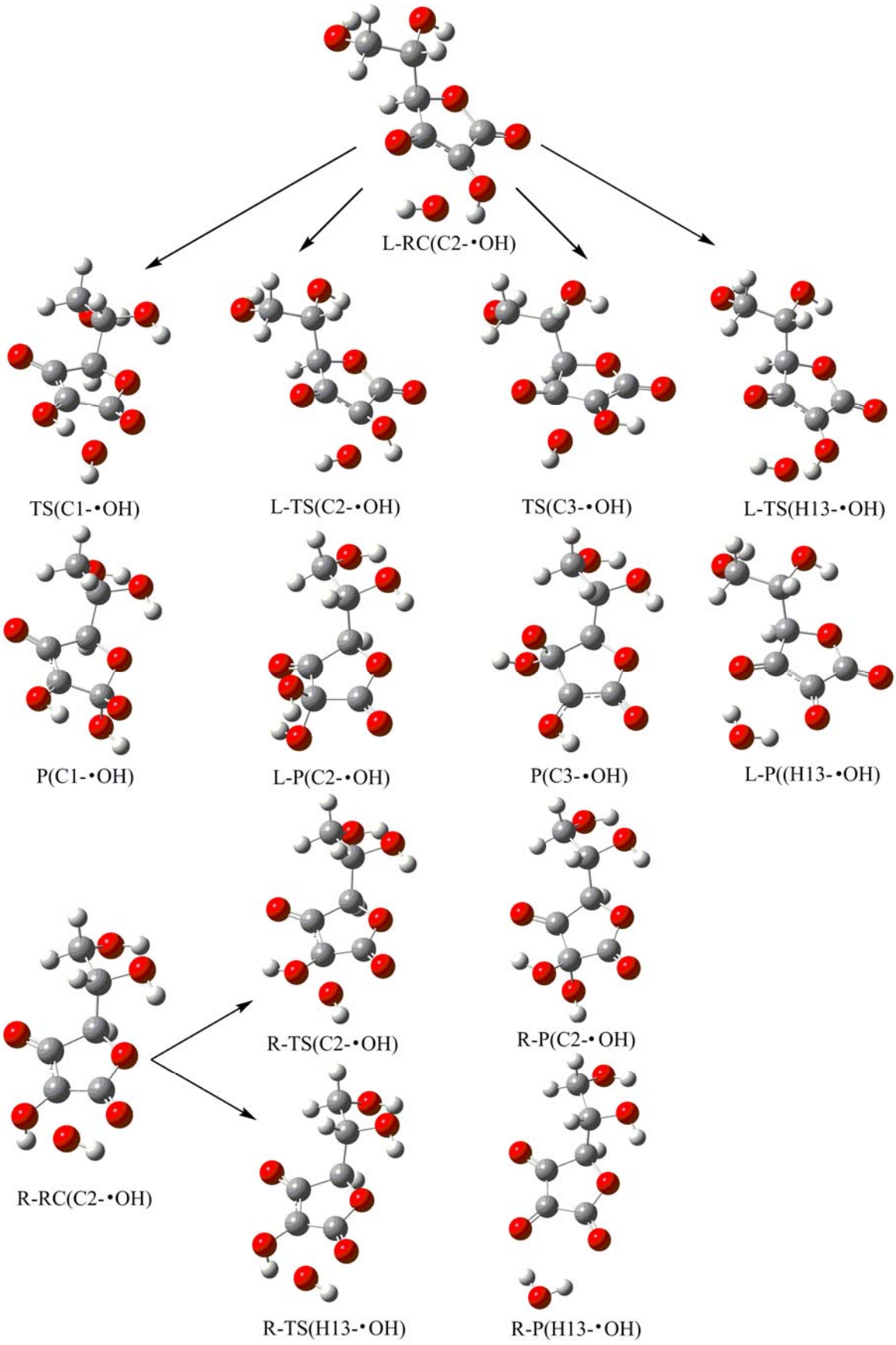


Fig. S1 The selected superposition of the optimized geometries in the gas phase and in solution at the B3LYP/6-311++G** level of theory. The red and yellow refer to the geometries in the gas phase and in solution, respectively.


RC(O8-•H)
TS(O8-•H)
P(O8-•H)
RC(O10-•H)
TS(O10-•H)
P(O10-•H)
TS(C1-•H)
P(C1-•H)
P(C2-•H)
TS(C3-•H)
P(C3-•H)


L-RC(C2-•OH)
TS(C1-•OH)
L-TS(C2-•OH)
TS(C3-•OH)
L-TS(H13-•OH)
P(C1-•OH)
L-P(C2-•OH)
P(C3-•OH)
L-P((H13-•OH)
R-RC(C2-•OH)
R-TS(C2-•OH)
R-P(C2-•OH)
R-TS(H13-•OH)
R-P(H13-•OH)

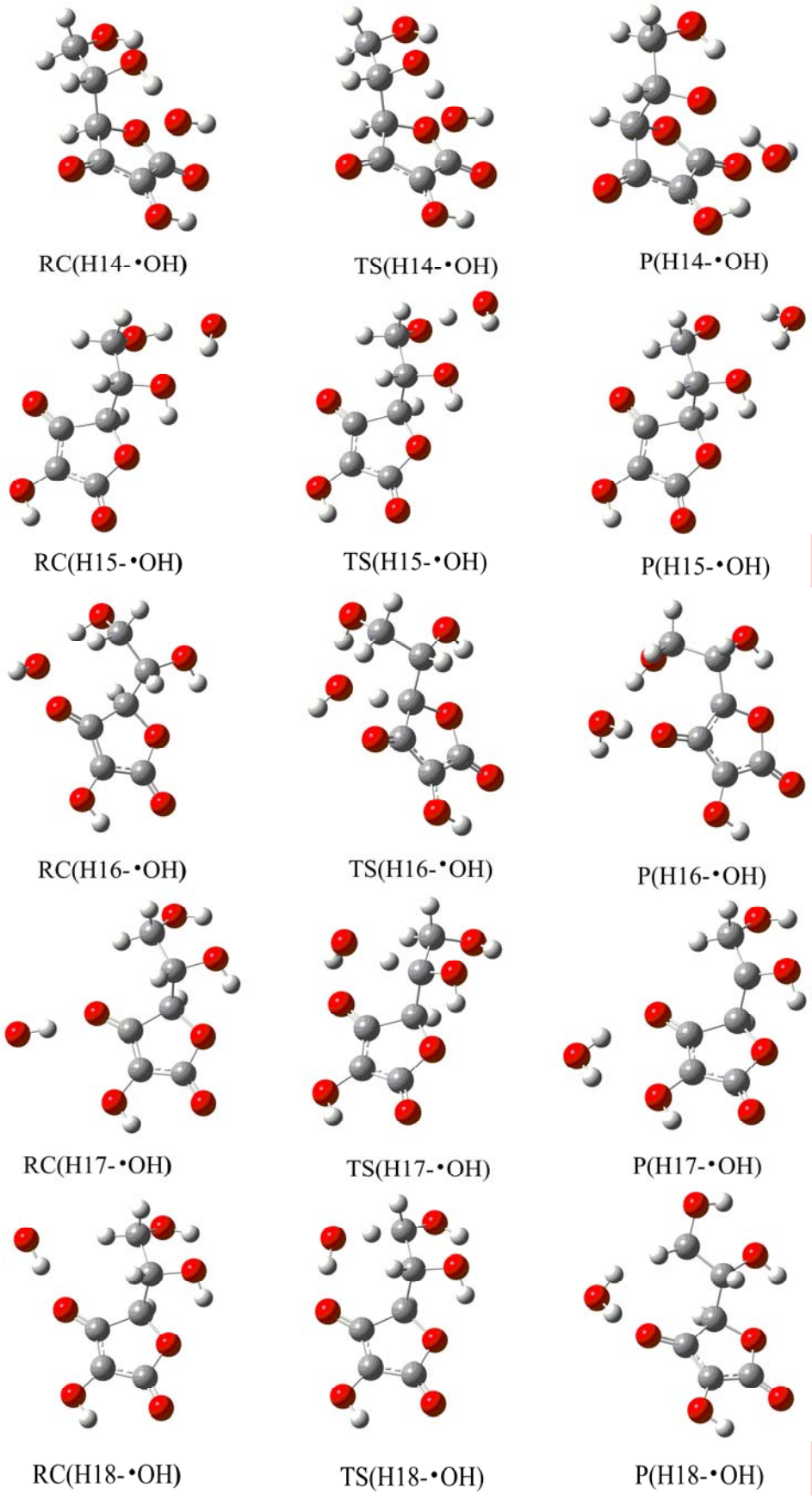


Fig. S2 All the optimized reaction complexes (RC), transition states (TS), and products (P) considered in the present study.

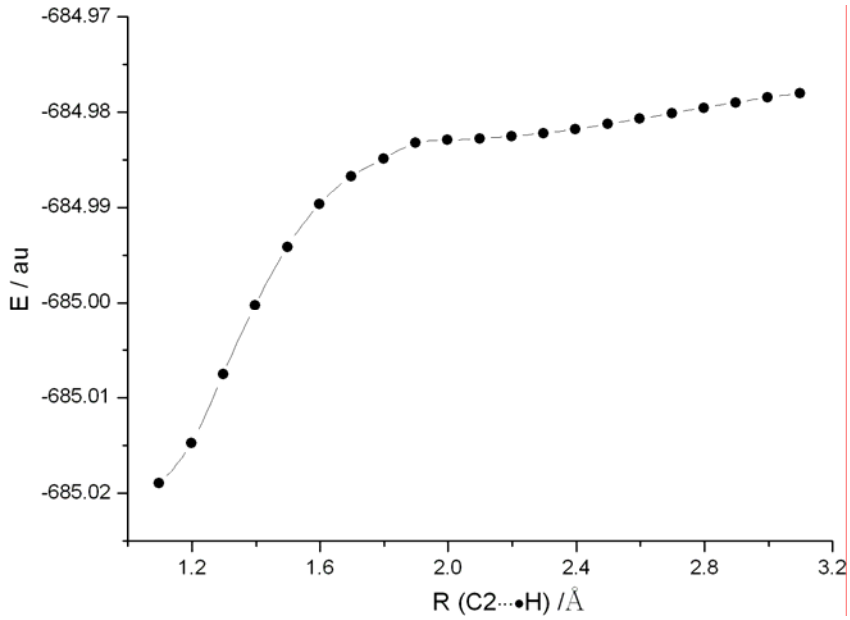


Fig. S3 The relaxed potential energy surface (PES) scan along the C2···•H distance of **P(C2-•H)**.

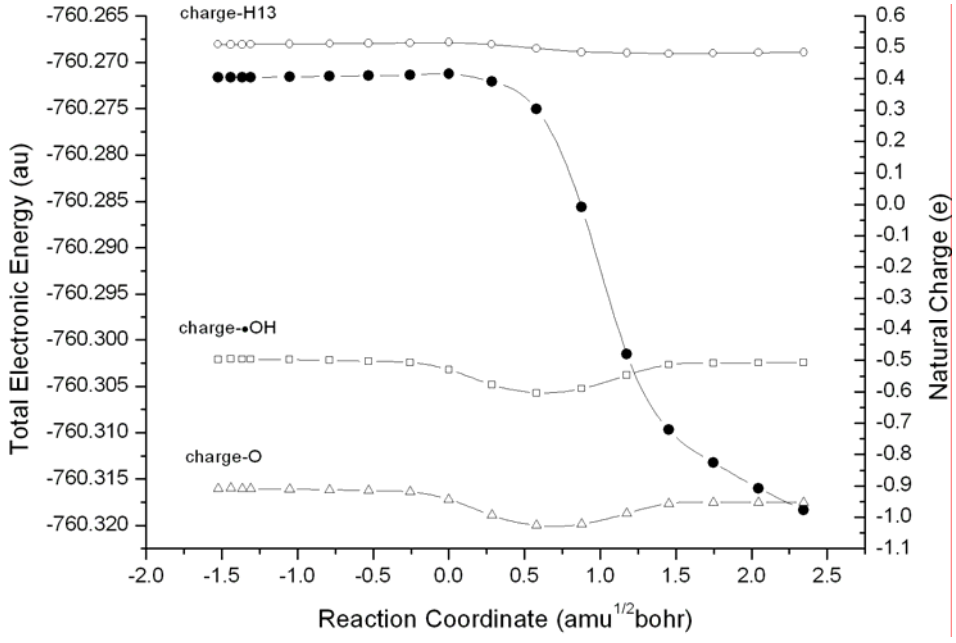


Fig. S4 The total electronic energies (solid dots) of H13 abstraction reaction starting from RC and the natural charges on H13, O atom of •OH, and •OH fragment along IRC.

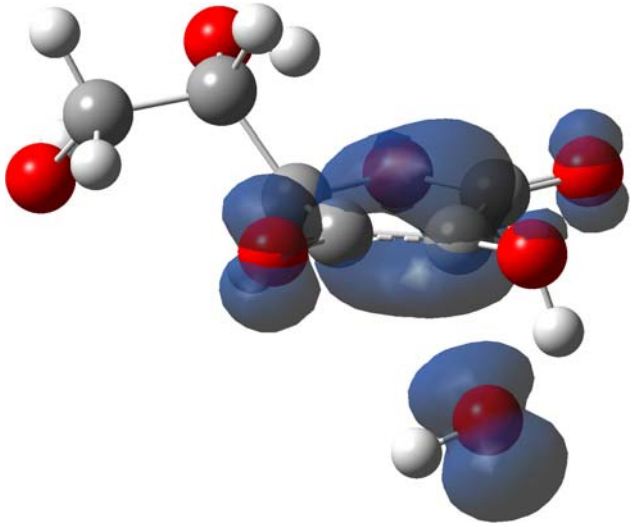


Fig. S5 The spin density distribution for **L-RC(C2-•OH)**. The isodensity contours are 0.003 electron bohr^{-3}.

Table S1 The calculated forward barrier heights (ΔE*, in kcal mol^{-1}) for the reactions of •H addition to neutral Vc at the B3LYP/6-311++G** level of theory [a]

Reaction sites	**C1**	**C2**	**C3**	**O8**
ΔE*	9.99	3.71	3.37	7.98

[a] All the barrier heights are corrected by ZPVE.

All the Cartesian coordinates of the geometries obtained at the B3LYP/6-311++G level of theory in the gas phase**

1. Reactants

Vitamin C (AAH^-)

C	-1.81760100	-0.86515000	-0.14879900
C	-1.85600900	0.53490800	0.01114200
C	-0.59658500	1.11256200	-0.14685700
C	0.33046600	-0.08784400	-0.44766000
C	1.42568600	-0.27793700	0.60663300
C	2.60857800	0.67008100	0.42711800
O	-0.50233600	-1.27042200	-0.43812300
O	-2.72173700	-1.69310200	-0.06918200
O	-3.04660700	1.18005400	0.30956500
O	-0.16940500	2.28288800	-0.07267100
H	-3.70685200	0.47496200	0.34783000
H	0.77655300	0.00220300	-1.44250500
H	0.98406500	-0.11438500	1.59857600
O	1.95817100	-1.61489300	0.54058700
H	1.20313400	-2.18133200	0.32677100
H	2.23395500	1.68426400	0.28323000
H	3.23091100	0.63638700	1.33317500
O	3.39210300	0.31864200	-0.71388700
H	3.42951400	-0.64714500	-0.70685500
C	0.76422218	3.33962482	0.55212705
H	1.12087661	2.33081482	0.55212705
H	1.12089502	3.84402301	1.42577855
H	1.12089502	3.84402301	-0.32152446
H	-0.30577782	3.33963801	0.55212705

Vitamin C (AAH_2)

C	-1.82011200	-0.93447500	-0.14086700
C	-1.83251700	0.51440400	0.02745900
O	-0.53274900	-1.32388900	-0.41162100
O	-2.75173200	-1.69366600	-0.06503500
C	-0.58645100	0.98196100	-0.13509500
O	-2.95717000	1.21994400	0.29821200
C	0.34251800	-0.16422300	-0.42068200
O	-0.11434400	2.24077400	-0.08209500
H	-3.69808900	0.59777400	0.33638600
H	-0.84177200	2.85375200	0.08930200
H	0.78766300	-0.09123800	-1.41633600
C	1.45182100	-0.41103200	0.61772000
H	1.00815800	-0.35473800	1.62198900

O	2.03447100	-1.69170700	0.40279100
H	1.32683600	-2.34211100	0.31701800
C	2.59900100	0.59348300	0.51522400
H	2.22698900	1.61191400	0.62778800
H	3.30152100	0.38608800	1.33184700
O	3.24729000	0.52809200	-0.74601800
H	3.55700200	-0.37853100	-0.86041900

•OH Radical

O	0.00000000	0.00000000	0.10842800
H	0.00000000	0.00000000	-0.86742600

2. Reaction Complexes

RC(O8-•H)

C	-1.80983900	-0.76615600	-0.20723400
C	-1.81364000	0.62448100	0.00256000
C	-0.53302900	1.16933400	-0.12650800
C	0.35990700	-0.04743800	-0.46012600
C	1.43915400	-0.30892700	0.59533500
C	2.65107400	0.60924200	0.45822800
O	-0.51091600	-1.20250500	-0.49779400
O	-2.74580900	-1.56916200	-0.16712800
O	-2.98226100	1.29706000	0.31522800
O	-0.07641300	2.32243000	-0.00656100
H	-3.66473800	0.61291100	0.34311100
H	0.81643400	0.06058600	-1.44814700
H	0.99387800	-0.16759600	1.58904800
O	1.93353400	-1.65597000	0.48421800
H	1.16354800	-2.19936200	0.26480700
H	2.30980300	1.63981100	0.35370900
H	3.26694700	0.51957300	1.36464600
O	3.42857600	0.28049100	-0.69324400
H	3.44459400	-0.68544800	-0.72122800
H	-2.46592500	-3.24243200	1.20276800

RC(O10-•H)

C	-1.78318900	-0.94290800	-0.15421700
C	-1.85152500	0.45808800	0.02664000
C	-0.60641800	1.05508300	-0.12463300
C	0.34532800	-0.11573100	-0.44165000
C	1.44822500	-0.29843400	0.60731600
C	2.61235100	0.67432800	0.43614800
O	-0.46282900	-1.31551900	-0.44655800
O	-2.67160000	-1.78553200	-0.08644800
O	-3.05264800	1.07005300	0.33451400
O	-0.18658100	2.23509500	-0.03710600

H	-3.70255900	0.35437000	0.34537100
H	0.78601700	-0.00228500	-1.43629300
H	1.00663400	-0.15664000	1.60257500
O	2.00637500	-1.62256800	0.52017600
H	1.26341900	-2.20443900	0.30671200
H	2.22037500	1.68452500	0.31302400
H	3.24090100	0.63529900	1.33749900
O	3.39297800	0.35783500	-0.71631100
H	3.45913600	-0.60629500	-0.72154300
H	-1.46811600	3.79800500	-0.39109900

L-RC(C2-•OH)

C	-1.53744700	1.07724000	-0.00057600
C	-1.69406200	-0.29402300	-0.39242500
C	-0.44462600	-0.95333000	-0.34696100
C	0.49912200	0.05385000	0.33833900
C	1.71489900	0.39320400	-0.53588600
C	2.82474800	-0.65408100	-0.46748600
O	-0.26415200	1.27118700	0.51013100
O	-2.33144100	1.99246200	-0.11359600
O	-2.75490500	-0.63977800	-1.16568500
O	-0.06613600	-2.04570100	-0.78939400
H	-3.36975900	0.10584100	-1.09665800
H	0.81143600	-0.29000800	1.32453200
H	1.38400600	0.48675300	-1.57941500
O	2.30356400	1.63307100	-0.10992300
H	1.56863100	2.20006600	0.16204900
H	2.39821100	-1.64343600	-0.63289100
H	3.55384000	-0.43693500	-1.26117000
O	3.46870700	-0.65668500	0.80375500
H	3.57328100	0.27384000	1.04191500
O	-2.35795300	-1.10535800	1.94318100
H	-2.07691500	-2.02685700	1.84384900

R-RC(C2-•OH)

C	-1.51750800	1.10856200	-0.11542400
C	-1.68892400	-0.31196700	-0.37160500
C	-0.42370100	-0.96928100	-0.27366000
C	0.54026400	0.08166500	0.29186300
C	1.79305400	0.29946200	-0.56531900
C	2.87553000	-0.75123700	-0.32934600
O	-0.20162500	1.32340100	0.31359300
O	-2.28079200	2.04200200	-0.20714600
O	-2.80580300	-0.83081200	-0.94068600
O	-0.08501000	-2.11560500	-0.56933000
H	-3.31713700	-1.09593800	-0.14622300

H	0.81515700	-0.16666300	1.32052400
H	1.50316400	0.27913500	-1.62452700
O	2.38815900	1.57139900	-0.26013900
H	1.65266500	2.17713100	-0.09248200
H	2.43424300	-1.74639100	-0.39002200
H	3.63990600	-0.64800700	-1.11277200
O	3.47047400	-0.61074100	0.95821100
H	3.59028600	0.33979700	1.08407400
O	-2.60928300	-0.86400500	1.59785800
H	-2.79952700	-0.00739800	2.00349400

RC(H14-•OH)

C	-1.22414700	-1.11521800	-0.46471300
C	-1.78297100	0.19753100	-0.21546600
C	-0.80746300	1.19186500	-0.50047000
C	0.47863500	0.39584300	-0.78572100
C	1.62635800	0.70258300	0.21029900
C	3.01610900	0.33816800	-0.32315500
O	0.09398700	-1.00399400	-0.78703200
O	-1.81859000	-2.17922200	-0.43328200
O	-3.10145300	0.37483700	-0.04229200
O	-0.88262100	2.41783400	-0.55595100
H	-3.47286500	-0.50753100	0.11067700
H	0.81530100	0.63832200	-1.79906500
H	1.59843900	1.80146300	0.32037600
O	1.49196800	0.04413700	1.43785400
H	0.50081200	0.02048800	1.74257600
H	3.15818000	0.71862600	-1.34032700
H	3.76071500	0.81818800	0.32965400
O	3.22401000	-1.06691600	-0.34998100
H	2.69764100	-1.40089800	0.39272100
O	-0.96551700	-0.01486800	2.04418100
H	-1.23162100	-0.92776100	2.21076100

RC(H15-•OH)

C	-2.07559300	-1.05720400	-0.16973400
C	-2.33718500	0.33995600	-0.04827600
C	-1.14734700	1.09230600	-0.14424200
C	-0.04410400	0.03689700	-0.35859600
C	1.02602700	0.01745300	0.74246500
C	2.06272900	1.13156100	0.55779600
O	-0.72609500	-1.25602200	-0.35757100
O	-2.87695600	-1.98016200	-0.12090000
O	-3.59942300	0.80272800	0.14631400
O	-0.94495600	2.31001600	-0.07050000
H	-4.16681800	0.01653200	0.16114700

H	0.43703100	0.15326400	-1.33159500
H	0.53247500	0.16912000	1.71481700
O	1.69854300	-1.24823900	0.75770500
H	1.02982600	-1.92139100	0.57690200
H	1.53654800	2.08622900	0.64359700
H	2.78051300	1.05309200	1.38747700
O	2.71723600	1.10781300	-0.68951300
H	3.41684000	0.40682200	-0.66038400
O	4.45801500	-0.97238300	-0.41241400
H	3.71550600	-1.43949100	0.00659800

RC(H16-•OH)

C	-2.12203200	-0.65203800	-0.29474900
C	-1.83083100	0.65920500	0.20069900
C	-0.46378500	0.88527700	0.21483500
C	0.16520900	-0.38766200	-0.35481700
C	1.11091900	-1.13579900	0.58995100
C	2.42076900	-0.38786300	0.86808700
O	-0.95217200	-1.27786900	-0.65817400
O	-3.21686900	-1.18286600	-0.41694600
O	-2.83620000	1.48197500	0.62704400
O	0.21419900	1.86781500	0.61465700
H	-3.65098100	0.97118900	0.51311000
H	0.67427400	-0.16473800	-1.29489900
H	0.59365900	-1.26384300	1.55517000
O	1.41817000	-2.42509600	0.05011200
H	0.58980900	-2.78432000	-0.29015100
H	2.18737600	0.45488600	1.52971300
H	3.06863700	-1.08543000	1.41095100
O	3.12304900	0.04266800	-0.27545500
H	2.71480400	0.88594100	-0.59092000
O	1.80612500	2.25890400	-1.14933100
H	1.69051100	2.97534800	-0.51227600

RC(H17-•OH)

C	-1.13190600	-1.82845800	-0.14764900
C	-1.68187800	-0.52911100	0.00030200
C	-0.71453100	0.44888000	-0.15469400
C	0.58338500	-0.32177900	-0.44298100
C	1.67299900	-0.09595200	0.61275700
C	2.43491600	1.21319200	0.42074100
O	0.23464000	-1.72689100	-0.42720100
O	-1.67886300	-2.91995400	-0.06132000
O	-3.01852400	-0.35312200	0.29029900
O	-0.72989100	1.70704900	-0.07992400
H	-3.38979200	-1.24426800	0.34085200

H	0.96994000	-0.08364200	-1.43795900
H	1.20128400	-0.09374400	1.60431200
O	2.65143600	-1.14852500	0.55327400
H	2.15831900	-1.95737300	0.35823800
H	1.72337100	2.02842800	0.28705700
H	3.03973500	1.40292900	1.31884000
O	3.27310300	1.16512400	-0.73290100
H	3.68162500	0.28967800	-0.71664100
O	-2.53537300	3.70536100	0.02223200
H	-1.93461900	2.90502600	-0.00123000

RC(H18-•OH)

C	-2.21819700	-0.61729200	-0.13603400
C	-1.87028200	0.75106500	-0.00887400
C	-0.50704800	0.94599900	-0.17277900
C	0.06428300	-0.46050600	-0.43575300
C	1.07684200	-0.93552500	0.62186500
C	2.51042100	-0.49368800	0.33375500
O	-1.06905500	-1.36473400	-0.40342600
O	-3.31474300	-1.15373000	-0.04451400
O	-2.83008600	1.70253700	0.25937600
O	0.20207300	1.98237400	-0.12951200
H	-3.66365700	1.21533400	0.31316600
H	0.50857300	-0.52462700	-1.43286900
H	0.77042800	-0.54876900	1.60265400
O	1.10956000	-2.37283100	0.66716900
H	0.20539200	-2.66446200	0.48305900
H	2.55597600	0.57941400	0.14983700
H	3.12579900	-0.72225000	1.21529900
O	3.03316900	-1.15824600	-0.81537900
H	2.75932400	-2.08027600	-0.72228000
O	2.58119500	3.21950300	0.11503700
H	1.70514700	2.76633900	-0.01195900

3. Transition States

TS(O8-•H)

C	-1.79340300	-0.77497300	-0.22529500
C	-1.82144300	0.59954800	-0.00310200
C	-0.53436100	1.15282800	-0.13285500
C	0.36619100	-0.06102400	-0.45004600
C	1.45039200	-0.30640300	0.60520200
C	2.65492600	0.61854900	0.45025100
O	-0.50278800	-1.22049700	-0.47427400
O	-2.73614600	-1.61915100	-0.13258200
O	-2.98167200	1.28356600	0.29214000

O	-0.09542300	2.31099400	-0.02566800
H	-3.66885800	0.60939500	0.37915900
H	0.81956200	0.03408200	-1.44100700
H	1.00777100	-0.15652200	1.59858600
O	1.95436300	-1.64869100	0.50564100
H	1.18585300	-2.21060000	0.33399300
H	2.30788000	1.64686600	0.34270900
H	3.27912300	0.53806600	1.35150200
O	3.42261300	0.28898600	-0.70707700
H	3.45738200	-0.67655800	-0.72467100
H	-2.81011900	-2.31754400	1.02934400

TS(O10-•H)

C	-1.81230900	-0.90480500	-0.16633400
C	-1.86451400	0.49996900	0.03648400
C	-0.60965600	1.06729600	-0.07338500
C	0.32786400	-0.08934200	-0.42174900
C	1.43661900	-0.32560100	0.61336500
C	2.62413100	0.62263100	0.45820500
O	-0.49750200	-1.28081800	-0.45539100
O	-2.71318600	-1.73404300	-0.11306800
O	-3.05399400	1.11800900	0.35387400
O	-0.19526100	2.27390300	0.01687000
H	-3.71244000	0.40978000	0.36237400
H	0.76385300	0.04927700	-1.41746300
H	1.00490700	-0.19954400	1.61487900
O	1.96370700	-1.65881400	0.48836100
H	1.20815100	-2.21998100	0.26490700
H	2.26081500	1.64519600	0.34973900
H	3.24811400	0.55529200	1.36112600
O	3.39897800	0.30454500	-0.69580900
H	3.43759500	-0.66082500	-0.71877000
H	-0.04573100	3.01766500	-1.25500600

TS(C1-•H)

C	1.83156500	-0.87164000	0.21577700
C	1.86155700	0.56016300	0.02771700
C	0.57253900	1.11430900	0.06742000
C	-0.34428200	-0.08690700	0.37809000
C	-1.49500000	-0.25339500	-0.62154300
C	-2.67733000	0.67324100	-0.35061300
O	0.47781800	-1.27056800	0.29459700
O	2.71927800	-1.68432200	-0.04155700
O	3.03782500	1.18406500	-0.23449500
O	0.15459800	2.27645100	-0.09678900
H	3.68560200	0.46709800	-0.32722200

H	-0.73456400	-0.01073400	1.39994500
H	-1.11224300	-0.05329800	-1.63094300
O	-2.00819900	-1.59578800	-0.56656600
H	-1.23945300	-2.16237400	-0.40793300
H	-2.31227900	1.69140300	-0.21302800
H	-3.35151500	0.64565800	-1.21905300
O	-3.38521400	0.29177300	0.82806100
H	-3.41175100	-0.67420500	0.80730200
H	2.01305200	-0.33106200	1.82383000

TS(C3-•H)

C	1.78068000	-0.88166100	0.14082200
C	1.82588900	0.51946700	-0.05390300
C	0.57482400	1.14022800	0.26129100
C	-0.35384800	-0.08042800	0.53263300
C	-1.37909500	-0.27413300	-0.59395100
C	-2.59120000	0.64579200	-0.46823500
O	0.50233800	-1.25393000	0.55523400
O	2.67438800	-1.71084200	-0.00352400
O	2.97006100	1.13880300	-0.45985000
O	0.12704000	2.27587200	0.01040000
H	3.64951300	0.44884500	-0.46202400
H	-0.85530400	-0.01624200	1.49724800
H	-0.88626900	-0.08357700	-1.55608400
O	-1.88593000	-1.62189600	-0.57916500
H	-1.13843500	-2.17859700	-0.31932000
H	-2.24817800	1.66581800	-0.29356300
H	-3.16005200	0.60983600	-1.40864300
O	-3.42885400	0.26226200	0.62239700
H	-3.45337700	-0.70349300	0.59612700
H	1.27626600	1.11966500	1.87037700

TS(C1-•OH)

C	1.69153100	-0.80132400	-0.13648100
C	1.67407300	0.66014400	-0.22847400
C	0.37045400	1.16820700	-0.04872700
C	-0.48148800	-0.08934000	0.22318100
C	-1.71860600	-0.19588100	-0.67467000
C	-2.89375600	0.66134600	-0.20955500
O	0.36060800	-1.22559400	-0.08100500
O	2.59200200	-1.51940900	-0.56188400
O	2.79712600	1.31692200	-0.55256500
O	-0.07645200	2.32388200	-0.10604000
H	3.44416400	0.61372300	-0.74299500
H	-0.75260200	-0.13602700	1.28148700
H	-1.44107700	0.10892000	-1.69285800

O	-2.19233600	-1.55266200	-0.69939000
H	-1.40152200	-2.10937000	-0.65779500
H	-2.54888700	1.67790700	-0.01816100
H	-3.64700400	0.68314600	-1.01068400
O	-3.47254900	0.15712600	0.99123100
H	-3.46861200	-0.80446600	0.89323600
O	1.88171500	-0.50258100	1.82174100
H	2.84139600	-0.43420900	1.89942300

L-TS(C2-•OH)

C	-1.52649300	1.09707400	-0.00982900
C	-1.74631400	-0.36731200	-0.13609900
C	-0.43553400	-0.96991800	-0.15544100
C	0.54005200	0.09546100	0.34153900
C	1.74925100	0.31534500	-0.57547500
C	2.83776300	-0.74056500	-0.39983300
O	-0.21322200	1.33280700	0.37090600
O	-2.29260900	2.01329300	-0.18283200
O	-2.71141800	-0.80253200	-1.02457000
O	-0.09686700	-2.14404500	-0.42601100
H	-3.53720300	-0.75637200	-0.52505200
H	0.87961900	-0.10778400	1.36293700
H	1.40177000	0.30109100	-1.61677500
O	2.36693800	1.58477200	-0.29502500
H	1.64293500	2.19719300	-0.10555800
H	2.38501000	-1.73184200	-0.43484000
H	3.55953300	-0.64208400	-1.22343700
O	3.50540800	-0.60191100	0.85372200
H	3.62436400	0.34928300	0.97574800
O	-2.58828600	-0.70861500	1.39996900
H	-2.22792400	-1.58013700	1.60852100

R-TS(C2-•OH)

C	-1.56448700	1.08352700	-0.09561500
C	-1.74660200	-0.36818400	-0.14109500
C	-0.44590400	-0.96019000	-0.18865400
C	0.52069300	0.10739400	0.30323700
C	1.75381900	0.30203500	-0.58405800
C	2.83771700	-0.74668100	-0.34708500
O	-0.24322500	1.34048000	0.26629700
O	-2.33597000	1.99347400	-0.29525700
O	-2.29818800	-0.67388900	1.65476700
O	-0.15224100	-2.12290000	-0.53896800
H	-3.13024400	-0.18172300	1.63644200
H	0.81640200	-0.06604000	1.34266000
H	1.43809900	0.25550600	-1.63458400

O	2.36021700	1.58005400	-0.32400800
H	1.62992400	2.19480500	-0.16896100
H	2.38982400	-1.74073600	-0.37099100
H	3.58252800	-0.66875600	-1.15225000
O	3.46785900	-0.57560900	0.92040400
H	3.58019200	0.37844800	1.02484700
O	-2.77847500	-0.89565300	-0.86634200
H	-2.59796900	-1.84656400	-0.89270700

TS(C3-•OH)

C	-1.62575600	1.08328100	0.10225400
C	-1.74651800	-0.25420100	-0.37010900
C	-0.52601800	-1.01915100	-0.12866800
C	0.44342400	0.06906500	0.40911800
C	1.54698800	0.41597600	-0.59646200
C	2.70637500	-0.57885300	-0.58155500
O	-0.35893100	1.27867800	0.60529900
O	-2.46913700	1.97214200	0.07371500
O	-2.88343500	-0.69656500	-0.94044900
O	-0.13679400	-2.05287000	-0.69588300
H	-3.52276800	0.02768600	-0.84849800
H	0.84868300	-0.21394300	1.37722900
H	1.11579000	0.43631000	-1.60598100
O	2.11334300	1.70642200	-0.29853200
H	1.38226200	2.24718900	0.03049400
H	2.30687100	-1.59246500	-0.61885300
H	3.32998300	-0.40337900	-1.47033000
O	3.49475700	-0.44960700	0.60004600
H	3.55551500	0.50097600	0.76325500
H	-1.75949800	-2.18625100	1.39506900
O	-1.26577900	-1.39730300	1.65207500

L-TS(H13-•OH)

C	-1.48012100	1.20372900	-0.02751400
C	-1.68566000	-0.18579400	-0.42155300
C	-0.44822600	-0.89490400	-0.33081400
C	0.54578200	0.08719200	0.30217200
C	1.80273600	0.32614100	-0.54413800
C	2.84952200	-0.77516700	-0.39525000
O	-0.15735600	1.34386500	0.41378800
O	-2.21248200	2.16039500	-0.05491000
O	-2.83459800	-0.63074200	-0.96016100
O	-0.14961200	-2.04411300	-0.66635100
H	-3.24239000	-1.04048700	-0.13981200
H	0.82103500	-0.23884600	1.30915200
H	1.50784000	0.39593600	-1.60006800

O	2.44114300	1.54962600	-0.14676400
H	1.72786600	2.16705800	0.06810200
H	2.37683300	-1.74739200	-0.53704400
H	3.61883000	-0.63289600	-1.16752100
O	3.44490700	-0.76156200	0.89967500
H	3.60519200	0.16987300	1.10068500
O	-2.74292100	-1.08799400	1.48452900
H	-2.23206300	-1.87623000	1.71064400

R-TS(H13-•OH)

C	-1.49847900	1.09684500	-0.14385700
C	-1.65709600	-0.32605200	-0.41567400
C	-0.39598500	-0.98197700	-0.26778600
C	0.55766200	0.07923300	0.29562900
C	1.81685200	0.29628800	-0.55273300
C	2.89938100	-0.75158300	-0.30486900
O	-0.18986600	1.31730000	0.30148500
O	-2.26334000	2.02580600	-0.25083800
O	-2.77774400	-0.86538500	-0.92978800
O	-0.05304900	-2.13618900	-0.52759800
H	-3.29800000	-0.99045000	-0.08605600
H	0.82626000	-0.15921700	1.32834700
H	1.53475900	0.27155500	-1.61408500
O	2.40709400	1.57003900	-0.24770300
H	1.66999600	2.17671200	-0.09127600
H	2.46121700	-1.74805200	-0.36690000
H	3.67019600	-0.64820100	-1.08185200
O	3.48230500	-0.60758700	0.98758600
H	3.60463500	0.34286000	1.11130400
O	-2.82407100	-0.77794200	1.56319100
H	-3.05371100	0.06993800	1.96556300

TS(H14-•OH)

C	-1.23105600	-1.08492100	-0.53866200
C	-1.79889200	0.21206700	-0.21161200
C	-0.82907700	1.23079500	-0.44463200
C	0.45122600	0.46572300	-0.80632300
C	1.61726000	0.70377900	0.19921900
C	2.99947000	0.34102900	-0.38334200
O	0.06490000	-0.93736500	-0.89644200
O	-1.82504900	-2.14843900	-0.54331800
O	-3.09536200	0.35857900	0.05914800
O	-0.92608900	2.45467300	-0.40949800
H	-3.44990300	-0.53801600	0.17434100
H	0.77052200	0.77152200	-1.80768000
H	1.60582600	1.80313800	0.33763900

O	1.47795800	0.00539200	1.38368500
H	0.37780600	-0.08442000	1.76025100
H	3.08872800	0.63972000	-1.43441300
H	3.75921800	0.89085500	0.19386300
O	3.23547300	-1.05444200	-0.29218700
H	2.70373600	-1.30807200	0.48474800
O	-0.82489300	-0.20792200	2.09328500
H	-0.96500900	-1.14937700	2.24597600

TS(H15-•OH)

C	-2.13417400	-1.00760400	-0.18515400
C	-2.32187900	0.40711500	-0.05924400
C	-1.08557400	1.08950700	-0.13116000
C	-0.04290100	-0.02337300	-0.33493400
C	1.01485900	-0.10540000	0.77317600
C	2.07762100	0.99007700	0.60568900
O	-0.80244100	-1.27746300	-0.34955700
O	-2.99360800	-1.87579400	-0.15114900
O	-3.55396500	0.93477700	0.11918600
O	-0.82274500	2.29344100	-0.04668400
H	-4.16673500	0.18223300	0.11788500
H	0.45774400	0.06922000	-1.30076500
H	0.51900500	0.03750800	1.74664800
O	1.65629500	-1.38334900	0.75714600
H	0.97574200	-2.04083000	0.56970600
H	1.56821400	1.95470700	0.73534700
H	2.80384600	0.87335200	1.42434200
O	2.70298600	0.98511900	-0.64147400
H	3.52854300	0.31449300	-0.61847100
O	4.47839600	-0.68902300	-0.50864200
H	3.94659400	-1.39427500	-0.11553000

TS(H16-•OH)

C	-1.97865200	0.84764700	0.24374100
C	-2.00260400	-0.55577500	-0.10648500
C	-0.66668300	-1.04786500	-0.29521900
C	0.20538800	0.09970900	0.09325000
C	1.27413000	0.54707300	-0.92170200
C	2.52423300	-0.35126800	-0.91400200
O	-0.70064700	1.25314700	0.35567000
O	-2.95671900	1.56234500	0.40890400
O	-3.15972200	-1.19154600	-0.32801700
O	-0.30402600	-2.16567400	-0.67836600
H	-3.85986600	-0.53116100	-0.18752300
H	0.75555900	-0.19428400	1.15719200
H	0.83893200	0.46287400	-1.93432600

O	1.66615900	1.89806700	-0.70193700
H	0.90150200	2.36391100	-0.34497800
H	2.17788800	-1.37827000	-1.10405700
H	3.13994900	-0.04264200	-1.76690800
O	3.33933200	-0.26508400	0.22703800
H	2.78958800	-0.43350600	1.03958000
O	1.58843800	-0.58847600	2.23483800
H	1.33906500	-1.50627800	2.39848400

TS(H17-•OH)

C	-1.90960800	-1.01791700	0.06096400
C	-1.98830600	0.35007300	-0.28725700
C	-0.74015700	0.86901400	-0.59525200
C	0.21328500	-0.34532200	-0.53144900
C	1.43040100	-0.14560300	0.39479800
C	2.70799600	0.25015400	-0.33627100
O	-0.57622700	-1.45596800	-0.06128200
O	-2.78455100	-1.78787200	0.43403500
O	-3.18798800	1.03266200	-0.21513500
O	-0.32082100	2.02272800	-0.85659500
H	-3.82718300	0.38853100	0.11752400
H	0.56641800	-0.59347700	-1.53792000
H	1.21529200	0.74363800	1.11193300
O	1.70511500	-1.30469000	1.15354100
H	0.86816100	-1.79524300	1.20263600
H	2.50243500	1.09358900	-0.99557800
H	3.45430800	0.55772100	0.40563300
O	3.20914000	-0.81911900	-1.14146100
H	3.17426200	-1.60557300	-0.58258300
O	1.10288100	2.18676500	1.59267800
H	0.58425200	2.45237100	0.79890700

TS(H18-•OH)

C	-2.12328600	-0.76775800	-0.24071600
C	-2.01169300	0.61102900	0.04178300
C	-0.69583000	1.04432000	-0.03116700
C	0.11589300	-0.21505500	-0.40649100
C	1.16514200	-0.62496100	0.66443700
C	2.58471000	-0.13583600	0.36844300
O	-0.84638900	-1.28690200	-0.52741100
O	-3.10870800	-1.49368200	-0.26248600
O	-3.12501100	1.36475500	0.36242400
O	-0.16497100	2.16583600	0.16041300
H	-3.86807300	0.74776500	0.32735400
H	0.59956200	-0.09398200	-1.38015000
H	0.84774100	-0.23677100	1.63854200

O	1.25685300	-2.05970700	0.72816000
H	0.38658500	-2.38416700	0.44510100
H	2.57962500	1.00475300	-0.00159100
H	3.19712100	-0.08508400	1.27789300
O	3.21222700	-0.90133000	-0.62212100
H	2.75546000	-1.75744700	-0.61557500
O	2.49804900	2.32821000	-0.32665000
H	1.51595400	2.39705500	-0.16794400

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P(O8-•H)

C	-1.81998300	-0.77750800	-0.41364100
C	-1.84935300	0.58324400	-0.06445500
C	-0.56361700	1.14335300	-0.08378100
C	0.35914400	-0.04344000	-0.42751400
C	1.46887600	-0.29050100	0.60102100
C	2.66829800	0.63851900	0.42901600
O	-0.48626800	-1.22184400	-0.47262200
O	-2.70039800	-1.71401800	0.07889000
O	-3.02216500	1.27028300	0.19135300
O	-0.13155500	2.30936600	0.09592200
H	-3.72605100	0.61016800	0.18319800
H	0.80206800	0.08628200	-1.42361000
H	1.04783900	-0.14667100	1.60444600
O	1.97036000	-1.63644600	0.48571800
H	1.19981600	-2.17894600	0.26431200
H	2.30913600	1.66207800	0.31301000
H	3.29903900	0.57500700	1.32788400
O	3.43584000	0.29919500	-0.72695800
H	3.43741000	-0.66704300	-0.75319000
H	-2.47595200	-1.91516700	1.02164600

P(O10-•H)

C	-1.81918300	-0.91914300	-0.16911700
C	-1.87230900	0.46177600	0.08291700
C	-0.59945400	1.03419700	0.12971300
C	0.33733500	-0.06160700	-0.33214900
C	1.50046800	-0.38498300	0.61735000
C	2.65210600	0.61524200	0.54341400
O	-0.46621700	-1.27017200	-0.41439200
O	-2.70694700	-1.78151000	-0.15284700
O	-3.07346700	1.07768900	0.40420200
O	-0.30487700	2.35448700	-0.24947000
H	-3.72777600	0.36472100	0.37693900
H	0.73417400	0.15880000	-1.33602000

H	1.09992500	-0.39897100	1.63860800
O	2.06436700	-1.67288200	0.30129600
H	1.30654300	-2.22330600	0.05543700
H	2.25823800	1.63303200	0.56773000
H	3.30869900	0.46887800	1.41328200
O	3.40377500	0.46558800	-0.66052500
H	3.42172800	-0.48711900	-0.82541400
H	-0.92838600	2.62547700	-0.94942600

P(C1-•H)

C	1.91806500	-0.86685400	0.52946500
C	1.85797200	0.59766200	0.14060200
C	0.55006900	1.13324900	0.10552600
C	-0.35849400	-0.09404500	0.35472400
C	-1.53073900	-0.16617000	-0.64024400
C	-2.74784100	0.66034600	-0.23385000
O	0.45215400	-1.25027100	0.15162400
O	2.88901900	-1.47960000	-0.07286900
O	3.00312600	1.07652300	-0.31052900
O	0.14387200	2.28689400	-0.12226900
H	3.51191300	0.20635200	-0.38847600
H	-0.75699700	-0.07369300	1.38286200
H	-1.17856400	0.18031200	-1.62081400
O	-1.97435000	-1.52691900	-0.74711700
H	-1.16790000	-2.05358800	-0.61215700
H	-2.43350700	1.67201300	0.02573600
H	-3.44017000	0.71291500	-1.08684800
O	-3.41208300	0.09637700	0.89649100
H	-3.36529500	-0.85999900	0.75877500
H	1.88242400	-0.99347600	1.64093400

P(C2-•H)

C	-1.91831000	-0.73710100	-0.35185900
C	-1.88391300	0.72717200	-0.04392200
C	-0.53849700	1.13173100	-0.47719200
C	0.30835900	-0.13071900	-0.57635100
C	1.28302500	-0.32689400	0.59215700
C	2.50901700	0.57849800	0.50288700
O	-0.63570900	-1.23160800	-0.54253200
O	-2.87362300	-1.48659200	-0.41570800
O	-2.09580700	0.93756400	1.47505900
O	-0.09396800	2.28669400	-0.70266600
H	-3.01395800	0.68373800	1.65135300
H	0.85058300	-0.18995800	-1.52559300
H	0.74377400	-0.11785300	1.52359900
O	1.78270300	-1.68294500	0.62176200

H	1.02779600	-2.24572700	0.40569500
H	2.19092100	1.59484100	0.26505800
H	3.02328100	0.57753200	1.47457300
O	3.40683600	0.14911000	-0.52179900
H	3.40415700	-0.81599300	-0.47160900
H	-2.70809900	1.27952000	-0.51032300

P(C3-•H)

C	1.76878700	-0.87278100	0.15778400
C	1.79471400	0.53574200	0.00511800
C	0.55105500	1.22743600	0.52296500
C	-0.36106500	-0.08653400	0.63913300
C	-1.29138300	-0.24098400	-0.56486300
C	-2.54494300	0.62195100	-0.45487000
O	0.54102600	-1.25044700	0.66657900
O	2.66228400	-1.68545800	-0.08550900
O	2.89204100	1.14328800	-0.47836300
O	0.02935700	2.25129700	-0.12877100
H	3.52071800	0.43116900	-0.68408700
H	-0.92975900	-0.12669900	1.56801200
H	-0.74829000	0.04888600	-1.47088800
O	-1.74361100	-1.60918100	-0.68393400
H	-1.00465800	-2.15831200	-0.38939700
H	-2.24051100	1.63487600	-0.19236700
H	-3.05264500	0.63429100	-1.43013000
O	-3.43635600	0.12590200	0.55009200
H	-3.42546700	-0.83440800	0.44285200
H	0.81969800	1.45800800	1.60365200

P(C1-•OH)

C	1.80000000	-0.71447500	0.07671400
C	1.63713300	0.78738100	-0.05820700
C	0.30800500	1.23201400	0.11367000
C	-0.50664900	-0.07045600	0.26593300
C	-1.72326700	-0.11059700	-0.67461100
C	-2.95846200	0.60192300	-0.12966600
O	0.36140700	-1.13823100	-0.12138400
O	2.65749900	-1.22141100	-0.72818500
O	2.70891600	1.46255500	-0.45050200
O	-0.17037100	2.37940800	0.11273500
H	3.32753200	0.73229800	-0.69558900
H	-0.83444800	-0.19959900	1.30691900
H	-1.44213400	0.35079600	-1.63094700
O	-2.10327200	-1.47597600	-0.90102000
H	-1.26590800	-1.96822500	-0.88110100
H	-2.68306400	1.59860500	0.21764000

H	-3.69490600	0.70008600	-0.94075700
O	-3.53437300	-0.10653000	0.96643700
H	-3.44831100	-1.04107800	0.73275500
O	2.07763200	-1.00111500	1.48587600
H	2.72117300	-1.71721200	1.41642100

L-P(C2-•OH)

C	1.57249900	1.06427600	-0.28494100
C	1.72716500	-0.38454500	0.15059900
C	0.42390400	-0.98766500	-0.21096700
C	-0.55382000	0.11884500	-0.50711100
C	-1.62967300	0.34655000	0.56128700
C	-2.70991900	-0.73301600	0.54650600
O	0.25148200	1.33999100	-0.55586700
O	2.41582000	1.92541400	-0.37576800
O	1.99486200	-0.40584100	1.59689100
O	0.26017900	-2.22811300	-0.46461200
H	2.91228100	-0.11387200	1.69849400
H	-1.02795600	0.00568700	-1.48910700
H	-1.13680000	0.35186400	1.54094400
O	-2.31299400	1.60454500	0.35932600
H	-1.63059800	2.23986500	0.10808100
H	-2.24006400	-1.71568200	0.47686200
H	-3.28545200	-0.67426400	1.48136800
O	-3.58483200	-0.58799900	-0.57215200
H	-3.71837900	0.36425100	-0.66843200
O	2.81268700	-1.03413500	-0.48782300
H	2.44839800	-1.91542000	-0.68040100

R-P(C2-•OH)

C	-1.55168100	1.09709400	-0.00545600
C	-1.79987400	-0.39781700	0.06335300
C	-0.43130900	-0.95612200	0.03255400
C	0.54214000	0.13604800	0.39543500
C	1.72375300	0.28306300	-0.56990700
C	2.80749200	-0.77013600	-0.35488600
O	-0.23670000	1.36966500	0.31305500
O	-2.32751000	1.99350400	-0.24468900
O	-2.52290400	-0.70323000	1.31352200
O	-0.14298900	-2.13179300	-0.37077700
H	-3.43508300	-0.41619300	1.16499200
H	0.92274200	0.08690800	1.42532400
H	1.34079900	0.19706600	-1.59432700
O	2.36266600	1.56404600	-0.40042900
H	1.65039600	2.19896400	-0.24774800
H	2.34149200	-1.75455000	-0.30225900

H	3.49945400	-0.74249200	-1.20923700
O	3.52516500	-0.54838400	0.85968300
H	3.64892500	0.40847700	0.91156500
O	-2.59960400	-0.87062200	-1.00583300
H	-2.17683400	-1.71644600	-1.23112300

P(C3-•OH)

C	1.74650200	1.10065900	-0.17439400
C	1.88898500	-0.30769000	-0.06661200
C	0.56343700	-1.01604400	0.09327100
C	-0.39090300	0.18724000	-0.35061100
C	-1.56566100	0.38790400	0.59350000
C	-2.70918000	-0.58963100	0.33815700
O	0.41552800	1.41690000	-0.30214700
O	2.63314000	1.95373600	-0.16780600
O	3.10281700	-0.85941600	0.09562600
O	0.39734400	-1.48284400	1.30779700
H	3.72889300	-0.11775600	0.13920100
H	-0.71293700	0.06337800	-1.38544600
H	-1.19832500	0.24128800	1.61320200
O	-2.13119500	1.71149100	0.44660700
H	-1.38325900	2.30516900	0.30253400
H	-2.31158200	-1.60006000	0.24569400
H	-3.39671400	-0.55807100	1.19527300
O	-3.41709500	-0.27905500	-0.86363800
H	-3.45682600	0.68646900	-0.88738500
H	0.49477900	-2.85792700	-0.42150500
O	0.37907300	-2.05295200	-0.94161700

L-P(H13-•OH)

C	0.98894000	1.83749600	-0.12333200
C	1.65710600	0.50831000	-0.05922100
C	0.63156500	-0.49475000	-0.24766100
C	-0.69138800	0.24173200	-0.44164200
C	-1.74222000	-0.07608700	0.63181200
C	-2.47218800	-1.39407800	0.38426600
O	-0.37828600	1.65181800	-0.35178900
O	1.43172000	2.95248700	-0.01131600
O	2.88946300	0.35164500	0.13785700
O	0.71502500	-1.73521200	-0.25007600
H	3.60236600	-1.52016300	0.25082100
H	-1.10957800	0.05396500	-1.43514200
H	-1.24255500	-0.12173400	1.60886600
O	-2.74991700	0.94674100	0.65827600
H	-2.29029100	1.78338100	0.50242000
H	-1.74449600	-2.18418100	0.19710400

H	-3.05476800	-1.64554200	1.28155500
O	-3.32901000	-1.31165100	-0.75208100
H	-3.77574000	-0.45820800	-0.67795200
O	3.52255500	-2.48973900	0.23722500
H	2.57176300	-2.57197500	0.06224500

R-P(H13-•OH)

C	-1.38292200	-0.76816600	-0.26044700
C	-1.40721200	0.70295700	-0.07100000
C	-0.03795200	1.17102600	-0.18287200
C	0.83100900	-0.06058800	-0.45463500
C	1.87509000	-0.33378200	0.63552900
C	3.11367600	0.55082500	0.51411600
O	-0.07640000	-1.18953600	-0.49023800
O	-2.27768900	-1.58536400	-0.24066900
O	-2.44835600	1.37417700	0.15414200
O	0.42704600	2.31038000	-0.07614500
H	-4.21256900	0.53308500	0.30846300
H	1.32018800	0.00392400	-1.43078400
H	1.41007600	-0.16418000	1.61610400
O	2.33727700	-1.69136900	0.55551400
H	1.56526000	-2.22828900	0.33017700
H	2.80821500	1.59207700	0.40707200
H	3.71224300	0.44212700	1.42936800
O	3.89388800	0.20514800	-0.62792600
H	3.92400400	-0.76046200	-0.63851400
O	-4.87696700	-0.17992700	0.32004900
H	-4.30795200	-0.93999600	0.13614400

P(H14-•OH)

C	0.81156600	-0.43700300	1.13609100
C	1.50110600	0.45439500	0.19886000
C	0.70062400	1.63276600	0.00542400
C	-0.65874300	1.19205600	0.55001700
C	-1.39606200	0.52154600	-0.67426900
C	-2.87002600	0.13179300	-0.35755600
O	-0.34766300	0.17335200	1.52156300
O	1.19840600	-1.48696600	1.61108300
O	2.62237100	0.14655500	-0.44033900
O	0.93939400	2.68318400	-0.58170400
H	2.52383100	-0.79947100	-0.73593500
H	-1.22670500	1.98361200	1.04048100
H	-1.43168500	1.32484300	-1.43946000
O	-0.69586300	-0.58468300	-1.05622500
H	0.69143200	-1.55358500	-1.44267200
H	-3.33635100	0.83863000	0.34061300

H	-3.43708300	0.16385600	-1.30164000
O	-2.92663800	-1.16825400	0.19789600
H	-2.08175800	-1.55514300	-0.11010900
O	1.51111600	-2.10940300	-1.37047200
H	1.35856600	-2.60634800	-0.55710400

P(H15-•OH)

C	-2.11796200	-1.05250400	-0.13503200
C	-2.30969600	0.35861300	-0.09061400
C	-1.09994200	1.03226400	-0.20599900
C	-0.05036100	-0.07924100	-0.36132800
C	0.99157800	-0.02801200	0.75230100
C	1.87310700	1.22477100	0.61287000
O	-0.76681100	-1.33683900	-0.28159100
O	-2.95689700	-1.93867800	-0.04534700
O	-3.56529100	0.89025200	0.06712900
O	-0.78561100	2.24675200	-0.17868900
H	-4.16338400	0.12961900	0.09149200
H	0.44571100	-0.03263500	-1.33428900
H	0.46283200	0.03487100	1.71446100
O	1.80867400	-1.20865000	0.75002300
H	1.20856900	-1.95310500	0.61318300
H	1.12058700	2.06191000	0.49508100
H	2.40918400	1.43296300	1.55868500
O	2.68325000	1.26297800	-0.46200500
H	4.19874800	-0.14387900	-0.83544800
O	4.45116500	-1.03547300	-0.55620800
H	3.64956700	-1.30783000	-0.08284800

P(H16-•OH)

C	-2.14260900	-0.68080200	-0.29304900
C	-1.83532900	0.61666300	0.16659700
C	-0.48533600	0.70414100	0.56667300
C	0.02042200	-0.62191800	0.31390300
C	1.32643200	-1.26880800	0.65103200
C	2.56338700	-0.40100800	0.36019100
O	-0.95274600	-1.45936900	-0.18045700
O	-3.17595200	-1.17339000	-0.73242400
O	-2.77099500	1.62141900	0.18657000
O	0.17559200	1.69228400	1.04009400
H	-3.58700900	1.22794400	-0.15016400
H	1.26645300	3.09369400	-1.38637700
H	1.34768200	-1.44878700	1.74390800
O	1.46636600	-2.53872800	0.00731400
H	0.63082400	-2.73772600	-0.43119900
H	2.54304800	0.45215200	1.04621300

H	3.43332900	-1.02406200	0.60109400
O	2.68512000	0.02333000	-0.98252800
H	2.40625400	0.95760100	-1.02801400
O	1.83258800	2.70639900	-0.71304900
H	1.19784100	2.41400400	0.00828100

P(H17-•OH)

C	-1.03231400	-1.76107000	-0.13997500
C	-1.55708400	-0.45610100	-0.03046800
C	-0.59571500	0.51605400	-0.27443200
C	0.69204000	-0.29140900	-0.57262800
C	1.80962300	-0.03245600	0.39727200
C	2.55773000	1.24236600	0.44288300
O	0.33145400	-1.68785900	-0.48371000
O	-1.57882300	-2.84622200	0.01175800
O	-2.89040700	-0.25323500	0.29789700
O	-0.61450800	1.76739000	-0.29175800
H	-3.27172600	-1.13647800	0.39176200
H	1.00381700	-0.09445200	-1.61030700
H	-3.54479400	1.87924800	0.31473600
O	2.54105600	-1.13237900	0.78924900
H	1.98707900	-1.90417700	0.58206500
H	1.89021100	2.06307300	0.18439500
H	2.95983600	1.40620300	1.45161900
O	3.66173100	1.29401500	-0.51109500
H	4.16627700	0.48356700	-0.38270000
O	-3.22082800	2.78138800	0.20202600
H	-2.27377900	2.61393700	0.01757100

P(H18-•OH)

C	2.19569600	-0.69216600	0.25393000
C	1.92662000	0.58127500	-0.30502700
C	0.59569600	0.93687700	-0.14803300
C	-0.04467000	-0.27656300	0.55352300
C	-1.08867800	-1.01058100	-0.29337800
C	-2.35162500	-0.24692000	-0.53125200
O	1.01979700	-1.22299000	0.79976500
O	3.25026900	-1.31315400	0.30947100
O	2.93475600	1.32101000	-0.89247200
O	-0.06454400	1.95906600	-0.46445100
H	3.73248300	0.78402000	-0.79270700
H	-0.47909600	0.00474100	1.51747500
H	-0.60384700	-1.26499900	-1.25465300
O	-1.47259400	-2.24572100	0.34643300
H	-0.64897100	-2.68595900	0.59223100
H	-2.70047700	2.15442800	1.08501700

H	-2.31677400	0.72705000	-0.99920400
O	-3.46042000	-0.99054800	-0.84451900
H	-3.31180100	-1.86915000	-0.46287300
O	-2.16735300	2.95557300	1.07150800
H	-1.38904600	2.69243400	0.53025700

All the Cartesian coordinates of the geometries obtained at the BHandHLYP/6-311++G level of theory in the gas phase**

1. Reactants

Vitamin C (AAH^-)

C	-1.79697700	-0.85839000	-0.14944500
C	-1.84243000	0.53391100	0.00807600
C	-0.58937600	1.09950200	-0.14023000
C	0.32443300	-0.09229000	-0.43868000
C	1.41589200	-0.27956800	0.60392500
C	2.58713500	0.66445400	0.41756800
O	-0.50368400	-1.25391000	-0.42119100
O	-2.69235000	-1.67611500	-0.07344900
O	-3.02371100	1.17223000	0.29847200
O	-0.15657300	2.25249100	-0.06068800
H	-3.68337300	0.48425100	0.33704500
H	0.76338400	-0.00290500	-1.42778100
H	0.98106900	-0.11500400	1.58961300
O	1.94116600	-1.59742300	0.53410000
H	1.20304000	-2.17329200	0.34521000
H	2.21379100	1.67177900	0.28476000
H	3.21326200	0.62622700	1.31040700
O	3.34833600	0.31964800	-0.71870600
H	3.41130200	-0.63212800	-0.71484400

•OH

O	0.00000000	0.00000000	0.10700900
H	0.00000000	0.00000000	-0.85607500

2. Reaction Complexes

RC(O8-•H)

C	1.79301400	0.75215500	-0.21215300
C	1.79678300	-0.63148300	0.00033500
C	0.52266300	-1.16060000	-0.11509900
C	-0.35406500	0.04856500	-0.45204900
C	-1.42850400	0.31386600	0.59112600
C	-2.63221500	-0.59691800	0.45127800
O	0.51346800	1.18105500	-0.48706400
O	2.71843300	1.54295800	-0.17779700

O	2.95721000	-1.29855100	0.30529400
O	0.05513000	-2.29417900	0.01388600
H	3.64050200	-0.63306700	0.31837300
H	-0.80465700	-0.06366700	-1.43343200
H	-0.99032000	0.17368200	1.57908700
O	-1.91094900	1.64397400	0.47286600
H	-1.15609400	2.19052300	0.26456200
H	-2.29489600	-1.62127000	0.35866700
H	-3.24996400	-0.49975100	1.34534400
O	-3.38896000	-0.27450400	-0.69428300
H	-3.42406900	0.67806800	-0.72801300
H	2.53878200	3.41594200	1.25156100

RC(O10-•H)

C	-1.75996700	-0.94249300	-0.15422900
C	-1.83749500	0.44888300	0.02221800
C	-0.59963100	1.04068900	-0.12071800
C	0.34148200	-0.12313500	-0.43490300
C	1.43942300	-0.29857100	0.60335200
C	2.58843400	0.67424100	0.42618000
O	-0.45980800	-1.30374200	-0.43094700
O	-2.63723600	-1.77858200	-0.08870200
O	-3.03128100	1.05509600	0.32135400
O	-0.18640300	2.20404000	-0.02755300
H	-3.67831600	0.35446700	0.34165000
H	0.77593700	-0.01082700	-1.42354400
H	1.00325400	-0.15651000	1.59192000
O	1.99458300	-1.60256800	0.51512400
H	1.27035800	-2.19475200	0.32374700
H	2.19292300	1.67513900	0.31049300
H	3.21913300	0.63609400	1.31568600
O	3.35105300	0.36418500	-0.71874800
H	3.44183500	-0.58522100	-0.72673200
H	-1.50585500	3.97649800	-0.34884300

L-RC(C2-•OH)

C	-1.51311500	1.09735000	-0.06954800
C	-1.68724000	-0.31991100	-0.32846200
C	-0.42877300	-0.95540400	-0.26642600
C	0.52245900	0.09028800	0.29843100
C	1.75269500	0.32752200	-0.56630000
C	2.82740000	-0.72435500	-0.37521000
O	-0.22010400	1.30536100	0.34395400
O	-2.26987000	2.01203200	-0.18100600
O	-2.78246600	-0.80282400	-0.95240300
O	-0.08221900	-2.09392500	-0.55174300

H	-3.39266300	-0.97527800	-0.23207800
H	0.81739400	-0.16787700	1.31090700
H	1.44663400	0.33438500	-1.61262300
O	2.34441800	1.57282400	-0.23779400
H	1.63107900	2.18336800	-0.06337300
H	2.38798100	-1.70925500	-0.46563900
H	3.58043900	-0.59631400	-1.15398300
O	3.42351900	-0.62455200	0.89700300
H	3.56465600	0.30556100	1.05396100
O	-2.52218500	-0.73881900	1.58188300
H	-2.00481400	-1.50828900	1.80877700

RC(H14-•OH)

C	-1.20327300	-1.08779100	-0.48417500
C	-1.77187100	0.21648900	-0.22391100
C	-0.79102700	1.20469800	-0.46552900
C	0.48359500	0.41776000	-0.75360500
C	1.61073800	0.68979000	0.25772200
C	2.98980200	0.35101800	-0.28419800
O	0.09421200	-0.95934600	-0.79094000
O	-1.78885400	-2.13765900	-0.48154100
O	-3.07121900	0.39288000	-0.03881200
O	-0.86184700	2.41680800	-0.48434100
H	-3.44321100	-0.46367300	0.16769000
H	0.82976300	0.68442600	-1.74851600
H	1.58078800	1.77392000	0.41402000
O	1.46954800	-0.01464200	1.43922800
H	0.48922400	-0.06750500	1.72766500
H	3.14723500	0.80511000	-1.25964700
H	3.72724700	0.76434700	0.40628200
O	3.17289100	-1.03449900	-0.41723000
H	2.65816400	-1.42569200	0.28801200
O	-0.97274700	-0.13792400	1.96625900
H	-1.23286600	-1.02768000	2.18568100

RC(H16-•OH)

C	-1.26291500	-1.75318500	-0.07185700
C	-1.60560100	-0.37996900	0.02348500
C	-0.51741200	0.40358200	-0.22289800
C	0.62575600	-0.56575300	-0.46826800
C	1.77495800	-0.48467500	0.52238600
C	2.40778100	0.90040900	0.60455900
O	0.06203600	-1.87569800	-0.37473500
O	-1.97627500	-2.71872300	0.07139800
O	-2.88532100	0.00994100	0.29677700
O	-0.34045900	1.64876600	-0.28120800

H	-3.39617800	-0.79164700	0.37912200
H	1.02042900	-0.44040000	-1.47120300
H	1.38118000	-0.74021700	1.50778000
O	2.76758700	-1.43079400	0.16612700
H	2.32541600	-2.26212600	0.01916300
H	1.90490100	1.45891400	1.39173600
H	3.44650700	0.76742900	0.88924100
O	2.37896800	1.62896400	-0.59158700
H	1.45999900	1.90672100	-0.69829600
O	-1.91461600	3.79047900	0.16864900
H	-1.41300800	2.95538800	0.01465700

RC(H17-•OH)

C	-1.12217500	-1.81019400	-0.12663000
C	-1.66971700	-0.51364800	-0.03708800
C	-0.69998100	0.44115300	-0.20615300
C	0.58514000	-0.34274400	-0.44017800
C	1.65189600	-0.08007700	0.61331700
C	2.41045900	1.21193900	0.38193100
O	0.22687900	-1.72306200	-0.36943900
O	-1.67110700	-2.88337800	-0.01602700
O	-3.00142800	-0.32105500	0.21232600
O	-0.70607700	1.68759900	-0.18182300
H	-3.38692200	-1.19078100	0.28097800
H	0.98316500	-0.14652100	-1.43090000
H	1.16910100	-0.03934800	1.58951200
O	2.61575300	-1.12113700	0.60420300
H	2.14177200	-1.93639500	0.45614600
H	1.70608900	2.01618200	0.21401300
H	3.00243000	1.43203800	1.27126100
O	3.24902500	1.11824600	-0.74703700
H	3.66995200	0.26404300	-0.69619900
O	-2.50194000	3.65391000	0.14444300
H	-1.90816100	2.87322900	0.03083000

RC(H18-•OH)

C	-1.12217500	-1.81019400	-0.12663000
C	-1.66971700	-0.51364800	-0.03708800
C	-0.69998100	0.44115300	-0.20615300
C	0.58514000	-0.34274400	-0.44017800
C	1.65189600	-0.08007700	0.61331700
C	2.41045900	1.21193900	0.38193100
O	0.22687900	-1.72306200	-0.36943900
O	-1.67110700	-2.88337800	-0.01602700
O	-3.00142800	-0.32105500	0.21232600
O	-0.70607700	1.68759900	-0.18182300

H	-3.38692200	-1.19078100	0.28097800
H	0.98316500	-0.14652100	-1.43090000
H	1.16910100	-0.03934800	1.58951200
O	2.61575300	-1.12113700	0.60420300
H	2.14177200	-1.93639500	0.45614600
H	1.70608900	2.01618200	0.21401300
H	3.00243000	1.43203800	1.27126100
O	3.24902500	1.11824600	-0.74703700
H	3.66995200	0.26404300	-0.69619900
O	-2.50194000	3.65391000	0.14444300
H	-1.90816100	2.87322900	0.03083000

3. Transition States

TS(O8-•H)

C	-1.77167600	-0.76837100	-0.22362800
C	-1.81093000	0.59400200	-0.00513300
C	-0.52861000	1.13803400	-0.12617600
C	0.36066500	-0.06572800	-0.44170700
C	1.44070800	-0.30680800	0.60281500
C	2.63291600	0.61521000	0.44101200
O	-0.50167100	-1.20445100	-0.45862000
O	-2.70327400	-1.60873700	-0.13211200
O	-2.96123300	1.27460800	0.27595600
O	-0.08988100	2.27849400	-0.01451600
H	-3.64063500	0.61860200	0.40920000
H	0.80710600	0.03137400	-1.42654800
H	1.00459200	-0.15659700	1.58990000
O	1.93864700	-1.62933800	0.49954600
H	1.18756900	-2.20275200	0.36229000
H	2.28714700	1.63655000	0.34613400
H	3.26170700	0.52956300	1.32805100
O	3.37663500	0.29444300	-0.71271300
H	3.43963000	-0.65698800	-0.73357900
H	-2.75933800	-2.27795000	0.98112900

TS(O10-•H)

C	-1.79017200	-0.90048900	-0.16503500
C	-1.84909900	0.49928400	0.03400800
C	-0.60278900	1.05102300	-0.06666700
C	0.32318900	-0.09704300	-0.41223300
C	1.42901700	-0.33210900	0.60888900
C	2.59979100	0.61972500	0.45461100
O	-0.49802500	-1.26751200	-0.43567100
O	-2.68314000	-1.71680400	-0.11378800
O	-3.02838600	1.10864700	0.34731200

O	-0.18286900	2.24701400	0.01058100
H	-3.68823100	0.41928700	0.34727100
H	0.75005900	0.04092700	-1.40319500
H	1.00335500	-0.21534700	1.60514800
O	1.95567800	-1.64260300	0.47045500
H	1.21980200	-2.21745800	0.27263700
H	2.23228800	1.63403400	0.36539300
H	3.22817200	0.54428100	1.34332900
O	3.35346500	0.32235600	-0.69731000
H	3.42398700	-0.62811700	-0.73125100
H	-0.16283300	2.97125600	-1.17339500

TS(C1-•H)

C	1.81196600	-0.86332900	0.21868600
C	1.84692900	0.55806600	0.02599900
C	0.56393000	1.10167000	0.05774400
C	-0.33913700	-0.09184000	0.36805900
C	-1.48624500	-0.25853800	-0.61798300
C	-2.65531300	0.66641200	-0.34417200
O	0.47836500	-1.25317100	0.27739200
O	2.69461700	-1.66735700	-0.03740500
O	3.01449000	1.17601300	-0.21614800
O	0.14579300	2.24777600	-0.10854300
H	3.65866800	0.47485100	-0.32097500
H	-0.72156000	-0.01435500	1.38415200
H	-1.11034300	-0.06294100	-1.62190500
O	-1.99313200	-1.58155400	-0.55283300
H	-1.24130400	-2.15540900	-0.41703400
H	-2.29132900	1.67838500	-0.22251400
H	-3.33377200	0.63102100	-1.19805500
O	-3.34006900	0.29824200	0.83132500
H	-3.39120200	-0.65425200	0.82083500
H	1.97754600	-0.33154400	1.77520300

TS(C3-•H)

C	1.75991600	-0.87534900	0.14154500
C	1.80695600	0.51741100	-0.06649500
C	0.56653700	1.12750200	0.26397100
C	-0.34840800	-0.08476700	0.52885400
C	-1.36474600	-0.27608200	-0.59092200
C	-2.56627500	0.63960500	-0.46214900
O	0.50475700	-1.23722100	0.54665000
O	2.64724700	-1.69132600	0.00505500
O	2.94344500	1.13151100	-0.45768300
O	0.11244500	2.24985400	0.01485200
H	3.62652700	0.46374900	-0.44314100

H	-0.84986900	-0.02473000	1.48464900
H	-0.87489600	-0.08375100	-1.54473300
O	-1.86540600	-1.60539000	-0.57567500
H	-1.13416000	-2.17161100	-0.33887000
H	-2.22389600	1.65216600	-0.29395800
H	-3.13504500	0.60141500	-1.39253400
O	-3.38719200	0.26014800	0.62012000
H	-3.43630300	-0.69194400	0.59356000
H	1.26138400	1.10417300	1.81964900

TS(C1-•OH)

C	1.66607200	-0.81313600	-0.14560600
C	1.66969000	0.63637700	-0.24579800
C	0.37370600	1.14446600	-0.07971000
C	-0.47153900	-0.09558500	0.21137900
C	-1.70465900	-0.21385700	-0.67037100
C	-2.85900300	0.66103900	-0.22169600
O	0.36027500	-1.21922500	-0.07808800
O	2.56294800	-1.54169400	-0.51141900
O	2.79167500	1.28257200	-0.54342300
O	-0.06500600	2.28483900	-0.15601100
H	3.44409900	0.59859100	-0.71030900
H	-0.72936900	-0.12250900	1.26468900
H	-1.43219600	0.06172500	-1.68948200
O	-2.18283100	-1.54836700	-0.65523000
H	-1.41642000	-2.11761000	-0.62176500
H	-2.50797500	1.67343000	-0.06865400
H	-3.61525600	0.66271100	-1.00844900
O	-3.41851800	0.20198900	0.98549500
H	-3.44444500	-0.74956600	0.92334900
O	1.81427000	-0.41173100	1.81871700
H	2.75345600	-0.30964900	1.94110900

L-TS(C2-•OH)

C	-1.51283400	1.08255800	-0.03083800
C	-1.72161900	-0.37279100	-0.16263100
C	-0.42887900	-0.96299200	-0.18330200
C	0.52925200	0.09852900	0.32524600
C	1.73843700	0.32290500	-0.57053200
C	2.81528800	-0.72838800	-0.38855000
O	-0.22435800	1.31393000	0.34486500
O	-2.27598300	1.98069800	-0.20787600
O	-2.71890100	-0.82094500	-0.97345000
O	-0.07913500	-2.11807600	-0.45951400
H	-3.49537100	-0.83832800	-0.41861800
H	0.85444400	-0.10722300	1.34171300

H	1.40504600	0.31323300	-1.60789800
O	2.34282300	1.57309900	-0.27668400
H	1.63613300	2.19272200	-0.11037000
H	2.36745500	-1.71209200	-0.44300500
H	3.54527700	-0.62118400	-1.19218500
O	3.45172700	-0.60136500	0.86265600
H	3.59259100	0.33241600	0.99606000
O	-2.53395200	-0.66679300	1.43425000
H	-2.12122100	-1.48285700	1.70397800

TS(C3-•OH)

C	-1.60463000	1.06803200	0.08223600
C	-1.72064300	-0.26229300	-0.39967700
C	-0.50887300	-1.00381300	-0.14097000
C	0.44128400	0.07496400	0.39414500
C	1.54759300	0.41358700	-0.59509500
C	2.69068500	-0.58327000	-0.56951700
O	-0.35710800	1.26387600	0.56769300
O	-2.44389100	1.93789200	0.05901900
O	-2.85211400	-0.71804000	-0.94244700
O	-0.12386500	-2.05925300	-0.63103000
H	-3.50765800	-0.03143900	-0.82284700
H	0.83454900	-0.20478800	1.35922700
H	1.12761300	0.43618600	-1.60073800
O	2.11028900	1.68192100	-0.29232000
H	1.39615000	2.23849300	0.00942600
H	2.28887400	-1.58680900	-0.61936900
H	3.32360700	-0.40718000	-1.44090900
O	3.45121500	-0.46560500	0.61037100
H	3.53895600	0.46907400	0.77838200
H	-1.79228300	-2.07443800	1.44287300
O	-1.31981400	-1.27608200	1.66211700

L-TS(H13-•OH)

C	-1.47124900	1.17222400	-0.05526400
C	-1.66767800	-0.21907100	-0.44143400
C	-0.42526200	-0.90347900	-0.33844700
C	0.53954700	0.09112900	0.28764500
C	1.79560300	0.33408500	-0.53739900
C	2.83598200	-0.75640700	-0.37446900
O	-0.17403400	1.32253000	0.36936200
O	-2.20834300	2.10562100	-0.09902800
O	-2.80930600	-0.69247200	-0.91222400
O	-0.11265500	-2.03454700	-0.66179300
H	-3.19124300	-1.01797000	-0.04006000
H	0.80048300	-0.22075900	1.29390000

H	1.51491000	0.40019100	-1.58900200
O	2.41376400	1.54315700	-0.13536300
H	1.71667400	2.16906800	0.04915200
H	2.37554500	-1.72343500	-0.52999100
H	3.61295000	-0.60718100	-1.12526600
O	3.39728800	-0.74283400	0.91626500
H	3.57388400	0.17105400	1.12396400
O	-2.72365200	-0.96933000	1.48630300
H	-2.30935900	-1.73885100	1.86535500

TS(H14-•OH)

C	-1.21390000	-1.05491500	-0.54482000
C	-1.79032900	0.24094600	-0.23612200
C	-0.80409300	1.24154900	-0.41255800
C	0.46621100	0.47356300	-0.75561400
C	1.60308700	0.68440000	0.26613700
C	2.97762100	0.36702800	-0.31259000
O	0.07035800	-0.90113000	-0.86969400
O	-1.80310500	-2.10019900	-0.57989700
O	-3.06917400	0.39373000	0.03400100
O	-0.88472600	2.45043600	-0.34884500
H	-3.42368100	-0.47749600	0.21441800
H	0.80373900	0.79275800	-1.73779300
H	1.58018100	1.76434200	0.46364800
O	1.46277000	-0.07000500	1.40388600
H	0.41982200	-0.18436800	1.72355000
H	3.10642200	0.80686800	-1.29949900
H	3.72445300	0.80363200	0.35362500
O	3.17567400	-1.01768000	-0.41975800
H	2.66643200	-1.38478500	0.30521900
O	-0.86330700	-0.33019200	1.99396500
H	-1.01687500	-1.23606100	2.24097600

TS(H16-•OH)

C	-1.95570600	0.86187300	0.22113100
C	-1.99521100	-0.54347700	-0.11954900
C	-0.64904400	-1.02788400	-0.31978400
C	0.22065400	0.09724800	0.08018100
C	1.28696000	0.52105500	-0.92792300
C	2.52036300	-0.37880200	-0.87419600
O	-0.69843100	1.24106200	0.28328200
O	-2.92544200	1.55724700	0.40658500
O	-3.13383100	-1.18679100	-0.27188500
O	-0.32426500	-2.13166000	-0.71280500
H	-3.83677000	-0.55733200	-0.09262000
H	0.75998300	-0.20576400	1.19034500

H	0.87901300	0.43013300	-1.94305200
O	1.67882300	1.85743200	-0.72470000
H	0.95335500	2.32490800	-0.32491300
H	2.17872600	-1.40083100	-1.05396900
H	3.15526700	-0.09235200	-1.71082100
O	3.29143200	-0.27773900	0.27571900
H	2.73674800	-0.42525700	1.07411600
O	1.52414500	-0.53992700	2.23746400
H	1.30613900	-1.41055800	2.55247700

TS(H17-•OH)

C	-1.88945000	-0.99859600	0.03080700
C	-1.96376600	0.36511500	-0.30596600
C	-0.71719200	0.87126800	-0.58991800
C	0.20994000	-0.34463000	-0.53832500
C	1.41728000	-0.16702000	0.37833400
C	2.66014100	0.33552600	-0.31760600
O	-0.58270700	-1.43241600	-0.08047200
O	-2.76314800	-1.75527300	0.39049300
O	-3.14928700	1.04725000	-0.22757100
O	-0.27926600	2.00953000	-0.81949500
H	-3.78642300	0.42702000	0.11753300
H	0.56238300	-0.58449000	-1.53899200
H	1.16621500	0.71463500	1.18055800
O	1.73341600	-1.33223800	1.06239800
H	0.92315700	-1.83515100	1.15006300
H	2.40771000	1.19695000	-0.92209200
H	3.38472400	0.63564800	0.43651300
O	3.20718700	-0.64918500	-1.16988600
H	3.23795700	-1.45832800	-0.66751900
O	0.99323500	1.89404200	1.75697800
H	0.52711400	2.28005900	1.00043800

TS(H18-•OH)

C	-2.10725500	-0.75513400	-0.23061400
C	-1.99391700	0.62045600	0.03238600
C	-0.68438500	1.03290800	-0.03947800
C	0.10568600	-0.22835500	-0.39879000
C	1.15091700	-0.62755300	0.66031900
C	2.55700300	-0.14737200	0.35581000
O	-0.85736800	-1.27617700	-0.49246900
O	-3.08908200	-1.46338300	-0.24524700
O	-3.09486200	1.37681800	0.33489000
O	-0.13982500	2.13434000	0.13934300
H	-3.83833600	0.77999000	0.30773700
H	0.57892900	-0.12278800	-1.37024900

H	0.84175900	-0.23630100	1.62667900
O	1.24749600	-2.04321700	0.72869700
H	0.38718300	-2.38631200	0.48793100
H	2.56465700	1.05225100	0.01380200
H	3.18368400	-0.11907200	1.24487800
O	3.14791800	-0.86270900	-0.66975200
H	2.74834800	-1.73209700	-0.65733300
O	2.51330200	2.26373300	-0.26894400
H	1.54486900	2.35937600	-0.14337200

4. Products

P(O8-•H)

C	-1.80731700	-0.77626000	-0.43900700
C	-1.83344000	0.58367300	-0.07745500
C	-0.56100400	1.12820000	-0.07656000
C	0.35117600	-0.04855200	-0.42607300
C	1.45425900	-0.29470900	0.59234800
C	2.64002500	0.63543200	0.42639400
O	-0.48383200	-1.20913500	-0.46613900
O	-2.66507700	-1.69728400	0.11701800
O	-3.00338500	1.26060300	0.16263800
O	-0.11651900	2.27624800	0.12234900
H	-3.69502700	0.60788200	0.19996100
H	0.79032800	0.08766000	-1.41408000
H	1.03607200	-0.15821800	1.58906400
O	1.95212600	-1.62154700	0.46770600
H	1.20239400	-2.16540000	0.23434600
H	2.27728000	1.65013500	0.32131000
H	3.26818600	0.56772700	1.31657800
O	3.39668100	0.30820300	-0.71901700
H	3.41886300	-0.64478900	-0.75383300
H	-2.40024000	-1.84841000	1.03233400

P(O10-•H)

C	-1.80275700	-0.90863900	-0.16111600
C	-1.85616000	0.45571300	0.09160500
C	-0.58366300	1.02210000	0.14961200
C	0.33387900	-0.07694600	-0.32035400
C	1.49386700	-0.40150800	0.60986200
C	2.62323900	0.60781500	0.54555100
O	-0.47023600	-1.25913900	-0.39127500
O	-2.68597500	-1.76113900	-0.16202800
O	-3.04476400	1.08066300	0.39241100
O	-0.29425200	2.32299400	-0.26292000
H	-3.70354900	0.38967300	0.36941300

H	0.71910900	0.14147100	-1.31964400
H	1.10152600	-0.43465900	1.62500800
O	2.05972500	-1.66086400	0.27264800
H	1.32349600	-2.22450100	0.04119500
H	2.21893600	1.61214300	0.59680600
H	3.28604900	0.45298000	1.39839800
O	3.35381000	0.49328800	-0.65472300
H	3.40208500	-0.44144300	-0.84078200
H	-0.94454200	2.58670100	-0.91425300

P(C1-•H)

C	1.88068200	-0.86676600	0.51033100
C	1.84159600	0.59347000	0.13458600
C	0.54332900	1.12127300	0.09255000
C	-0.35204300	-0.09484300	0.35414500
C	-1.51140600	-0.19062400	-0.63344900
C	-2.71252700	0.65326200	-0.25705900
O	0.46057300	-1.23150500	0.17125700
O	2.82912600	-1.48661200	-0.10636400
O	2.98413300	1.08714200	-0.27032800
O	0.13805400	2.25919200	-0.14010900
H	3.50528000	0.25461200	-0.36791900
H	-0.74744900	-0.06252300	1.37342700
H	-1.15556600	0.12131100	-1.61508300
O	-1.95954100	-1.53227400	-0.69646800
H	-1.17375200	-2.06922300	-0.58040800
H	-2.39327800	1.66494600	-0.04060800
H	-3.40225600	0.67627100	-1.10229600
O	-3.36576800	0.14188400	0.88273200
H	-3.35481300	-0.80737000	0.78371200
H	1.89142200	-0.97526400	1.61678500

P(C2-•H)

C	-1.88174500	-0.75192100	-0.33938800
C	-1.87789900	0.72644000	-0.06344200
C	-0.52554000	1.12341400	-0.45978900
C	0.31239100	-0.12629100	-0.56458100
C	1.28272800	-0.34593800	0.58787000
C	2.48565200	0.57437800	0.51757100
O	-0.62966200	-1.21491000	-0.53493200
O	-2.82376000	-1.49321400	-0.36357900
O	-2.17351300	0.93281000	1.37030500
O	-0.06802800	2.28304000	-0.63154300
H	-3.09023500	0.70027000	1.50478300
H	0.85071600	-0.19051300	-1.50733500
H	0.74659000	-0.16494400	1.51783800

O	1.79195200	-1.67794600	0.58230700
H	1.06060900	-2.25288800	0.37457000
H	2.14977800	1.58207700	0.30527900
H	2.99845600	0.55913600	1.48052100
O	3.37552100	0.18259400	-0.50530900
H	3.40596300	-0.77013300	-0.47685600
H	-2.67546100	1.23750100	-0.60624500

P(C3-•H)

C	1.79872100	0.87130100	-0.08844300
C	1.86068100	-0.53160700	-0.29399100
C	0.51230400	-1.18209000	-0.15358800
C	-0.34550400	0.12009600	-0.38010000
C	-1.52743200	0.21069500	0.55098500
C	-2.64474400	-0.73699100	0.17699100
O	0.50905300	1.26103800	-0.08188900
O	2.72872300	1.64124700	0.04766200
O	3.03780500	-1.15375300	-0.31569500
O	0.37319800	-1.73802900	1.04628100
H	3.70504700	-0.49100200	-0.13202600
H	-0.64941200	0.23370000	-1.41715100
H	-1.17332600	-0.04287500	1.54387700
O	-2.09240600	1.52256800	0.52659200
H	-1.36423600	2.13704500	0.54253000
H	-2.24470700	-1.73496900	0.05561700
H	-3.37359800	-0.75336500	0.98771400
O	-3.27707100	-0.35709500	-1.02958400
H	-3.36502100	0.59174100	-0.98954800
H	0.30668000	-1.85650100	-1.00906700

P(C1-•OH)

C	1.76971100	-0.71113500	0.07746400
C	1.62384000	0.78648500	-0.05444700
C	0.30115800	1.22155800	0.10172000
C	-0.49788000	-0.07472400	0.25621400
C	-1.70693300	-0.12736900	-0.67202100
C	-2.92655600	0.59594600	-0.13691600
O	0.37089200	-1.11870700	-0.12908100
O	2.62944200	-1.21290900	-0.71897400
O	2.69351400	1.45391400	-0.41895500
O	-0.17964900	2.35240300	0.08788800
H	3.30789500	0.74349000	-0.67091000
H	-0.81663200	-0.20411800	1.29089200
H	-1.42819100	0.31432200	-1.62887600
O	-2.08818700	-1.47684800	-0.86851600
H	-1.27136100	-1.97752000	-0.87228000

H	-2.64917500	1.59381900	0.17888500
H	-3.66452600	0.67304500	-0.93712800
O	-3.48388800	-0.07760400	0.96820100
H	-3.42881000	-1.00785900	0.76231500
O	2.04498900	-0.99202400	1.45976700
H	2.67384700	-1.70553700	1.40237300

L-P(C2-•OH)

C	1.53155100	1.06462700	-0.26293900
C	1.75012800	-0.38212900	0.17366000
C	0.39916500	-1.01790500	0.03153900
C	-0.55418500	0.06229500	-0.41486000
C	-1.66848000	0.39129400	0.56266700
C	-2.73695400	-0.68498700	0.59965500
O	0.24080700	1.27434700	-0.54281700
O	2.34374800	1.93534800	-0.33307900
O	2.23714700	-0.36041200	1.50005500
O	0.32846600	-2.21594400	-0.41504300
H	3.11135700	0.02140100	1.46029100
H	-0.97006400	-0.15208500	-1.39642900
H	-1.22564600	0.48785900	1.55263000
O	-2.32928200	1.60356600	0.21310100
H	-1.65606400	2.22005300	-0.06112200
H	-2.26441600	-1.65912600	0.64052700
H	-3.34644400	-0.54758400	1.49392400
O	-3.55309900	-0.64400500	-0.54849200
H	-3.69430100	0.27959600	-0.73995500
O	2.66846700	-1.01693500	-0.65426000
H	2.22819800	-1.85701000	-0.84391400

P(C3-•OH)

C	1.73771500	1.08869100	-0.16474500
C	1.87283200	-0.31562300	-0.05437900
C	0.54072400	-1.00914400	0.08564300
C	-0.38050800	0.20060200	-0.34925300
C	-1.54718700	0.41652300	0.58471000
C	-2.67281800	-0.57142500	0.35760300
O	0.43320200	1.40388000	-0.29113200
O	2.62303400	1.91998100	-0.15364100
O	3.06624900	-0.87248700	0.11161000
O	0.33560500	-1.48743300	1.27791000
H	3.70447300	-0.15840900	0.14132500
H	-0.70249900	0.08887200	-1.37722900
H	-1.18090300	0.30114800	1.59918600
O	-2.11291700	1.71362600	0.39858300
H	-1.38653500	2.31873700	0.27768700

H	-2.26797400	-1.57303800	0.30728200
H	-3.36080800	-0.51524600	1.20214100
O	-3.36523400	-0.30832400	-0.84421000
H	-3.43543300	0.64114600	-0.90190700
H	0.40532500	-2.81663400	-0.43476500
O	0.38503800	-2.01228400	-0.94551900

L-P(H13-•OH)

C	0.97193600	1.82548600	-0.12289700
C	1.64007300	0.50745700	-0.06004400
C	0.62620200	-0.48548400	-0.24187900
C	-0.68570200	0.24866500	-0.43475300
C	-1.72961800	-0.07182100	0.62718300
C	-2.44257900	-1.38634300	0.37844500
O	-0.37093900	1.63774300	-0.33713500
O	1.41327200	2.92684000	-0.01439200
O	2.86277100	0.35494500	0.13201500
O	0.70450000	-1.71214800	-0.24019400
H	3.58139500	-1.52199000	0.24635500
H	-1.09684300	0.06384900	-1.42261200
H	-1.23591700	-0.11356000	1.59823300
O	-2.72986800	0.93120300	0.64542700
H	-2.29232100	1.76957900	0.51546100
H	-1.71367400	-2.16686400	0.20288000
H	-3.02729300	-1.63635800	1.26426400
O	-3.27914900	-1.30953500	-0.75177900
H	-3.74779700	-0.48184800	-0.68398600
O	3.48727000	-2.47701600	0.23333500
H	2.54771100	-2.55682600	0.06486100

P(H14-•OH)

C	0.81480700	-0.44694900	1.14647800
C	1.52376500	0.43861400	0.21720700
C	0.71110000	1.59830200	-0.00236700
C	-0.63622700	1.16669400	0.53574400
C	-1.38926000	0.51281600	-0.66758600
C	-2.85671400	0.17100500	-0.33275100
O	-0.32885800	0.15332100	1.49605900
O	1.20284000	-1.47622000	1.62140400
O	2.63089400	0.12251500	-0.40928700
O	0.95719500	2.62713600	-0.59094700
H	2.51950900	-0.79782700	-0.73034000
H	-1.18553300	1.95817000	1.02935700
H	-1.41372600	1.30815900	-1.43036800
O	-0.73260600	-0.60330700	-1.04779700
H	0.63787500	-1.48550000	-1.45454600

H	-3.29459700	0.89016200	0.35938600
H	-3.43045800	0.20966500	-1.26262200
O	-2.93626200	-1.10905900	0.22499600
H	-2.12393200	-1.52127800	-0.09736800
O	1.45655400	-2.03377800	-1.42844300
H	1.28798500	-2.64931500	-0.72173700

P(H15-•OH)

C	-2.04598600	-1.07718200	-0.12606400
C	-2.31484500	0.30308700	-0.09362200
C	-1.15622700	1.04006000	-0.21163900
C	-0.05767500	-0.01304900	-0.36728100
C	0.97848200	0.06680700	0.73716300
C	1.86923300	1.28646600	0.59611100
O	-0.69301100	-1.28436600	-0.28764200
O	-2.81130100	-2.01206000	-0.02612100
O	-3.59426200	0.76551900	0.07873900
O	-0.89670500	2.25116900	-0.18825300
H	-4.14378900	-0.01177400	0.14210500
H	0.42579200	0.06748100	-1.33653300
H	0.45274600	0.14730000	1.68951000
O	1.78652300	-1.09827200	0.75221100
H	1.20139900	-1.83831300	0.60128100
H	1.20364100	2.15600100	0.47807600
H	2.46971800	1.44976100	1.49405800
O	2.67305400	1.28628100	-0.50515100
H	4.26809700	-0.37298700	-1.00482400
O	4.40069100	-1.15616200	-0.48040700
H	3.56458700	-1.25146500	-0.01868700

P(H16-•OH)

C	-2.13900800	-0.65234500	-0.28329000
C	-1.82007700	0.64503600	0.15600700
C	-0.48007000	0.71857700	0.53265600
C	0.00488500	-0.60947900	0.27442800
C	1.27873600	-1.28766200	0.63952100
C	2.52650200	-0.44823200	0.39440700
O	-0.98942400	-1.42583500	-0.18760700
O	-3.17981500	-1.11915700	-0.69306900
O	-2.74529300	1.64129500	0.18040300
O	0.19832900	1.68289100	0.99027100
H	-3.56147400	1.25958300	-0.13306200
H	1.41614900	3.10504200	-1.35959100
H	1.25932500	-1.48270800	1.72064400
O	1.40803500	-2.52808400	-0.02230300
H	0.56610700	-2.75533500	-0.40450500

H	2.49662200	0.40209300	1.07029900
H	3.37366600	-1.07669400	0.66375000
O	2.68944700	-0.03613700	-0.93132600
H	2.45451800	0.89405100	-0.99429100
O	1.93039200	2.66822200	-0.69137800
H	1.27590200	2.39304500	-0.00553500

P(H17-•OH)

C	-1.02100200	-1.74576600	-0.13117500
C	-1.55149500	-0.44946300	-0.03323700
C	-0.58980000	0.50875300	-0.26336300
C	0.68155200	-0.29636500	-0.54820500
C	1.79289800	-0.02972700	0.41655600
C	2.52970100	1.25259500	0.43044700
O	0.31993800	-1.67077800	-0.44863700
O	-1.56468900	-2.81743600	0.01871800
O	-2.87604600	-0.24838700	0.27789700
O	-0.59834800	1.74714000	-0.27666600
H	-3.26178700	-1.11479600	0.38085800
H	1.00112700	-0.10691900	-1.57555600
H	-3.50889400	1.83273700	0.29489500
O	2.57477500	-1.10322400	0.73167000
H	2.05456900	-1.88852200	0.55726800
H	1.85701500	2.05514100	0.16147300
H	2.92387900	1.43801800	1.42975200
O	3.60808700	1.27023800	-0.50907200
H	4.10415900	0.46887800	-0.37792900
O	-3.20787200	2.73202800	0.19185800
H	-2.26795500	2.59866300	0.01695800

P(H18-•OH)

C	2.18009500	-0.68001100	0.25474700
C	1.91103300	0.58848300	-0.29779000
C	0.58566100	0.91997100	-0.15227800
C	-0.03614500	-0.28958000	0.54174600
C	-1.07436900	-1.01791900	-0.29507500
C	-2.33768900	-0.25686500	-0.50576400
O	1.02436200	-1.21354700	0.77372300
O	3.22830400	-1.28410700	0.31231900
O	2.90874900	1.33023300	-0.87089400
O	-0.08843600	1.91567800	-0.46940500
H	3.70588000	0.81541000	-0.77276800
H	-0.46346700	-0.01173400	1.50086500
H	-0.60762600	-1.25174900	-1.25957000
O	-1.43656200	-2.24182900	0.33062200
H	-0.62611900	-2.67946400	0.57755200

H	-2.69799500	2.18165300	1.05861900
H	-2.30568200	0.71050900	-0.97045700
O	-3.43610000	-0.99588300	-0.80731100
H	-3.29981300	-1.86371200	-0.42934400
O	-2.16097000	2.96577100	1.04418000
H	-1.39146300	2.70409400	0.51569100