

Article

# Antioxidant Properties of the Vam3 Derivative of Resveratrol

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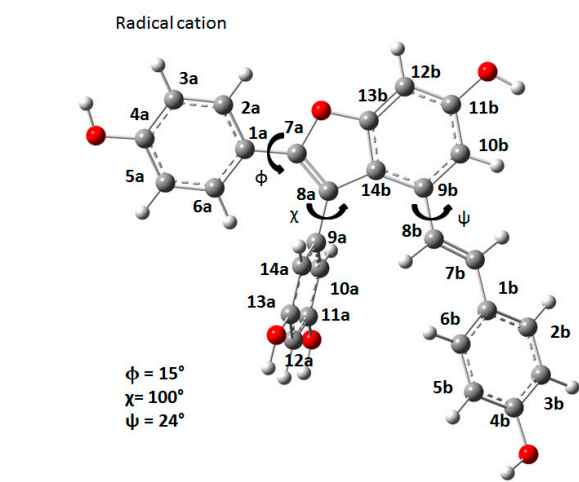
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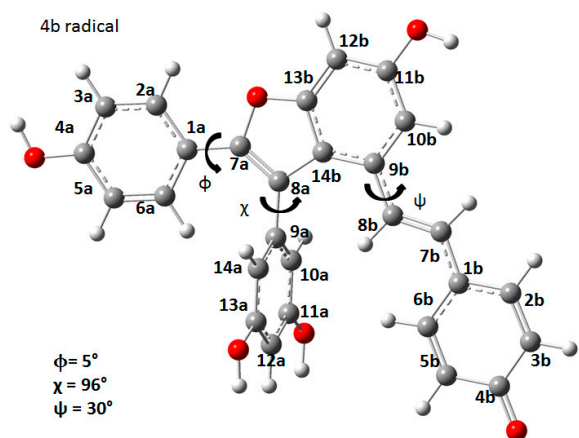
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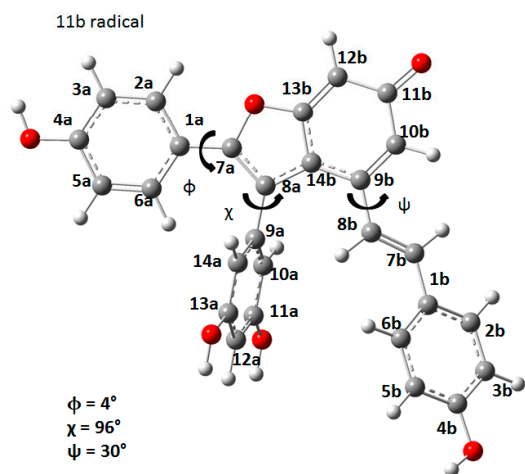
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Bond type	Distance (Å)	Bond type	Distance (Å)
1a-2a	1.405	1b-2b	1.407
2a-3a	1.390	2b-3b	1.388
3a-4a	1.395	3b-4b	1.394
4a-5a	1.396	4b-5b	1.398
5a-6a	1.387	5b-6b	1.389
6a-1a	1.407	6b-1b	1.405
1a-7a	1.460	1b-7b	1.463
7a-8a	1.372	7b-8b	1.347
8a-9a	1.486	8b-9b	1.464
9a-10a	1.398	9b-10b	1.404
10a-11a	1.393	10b-11b	1.400
11a-12a	1.397	11b-12b	1.393
12a-13a	1.396	12b-13b	1.383
13a-14a	1.394	13b-14b	1.405
14a-9a	1.398	14b-9b	1.417
8a-14b	1.452		

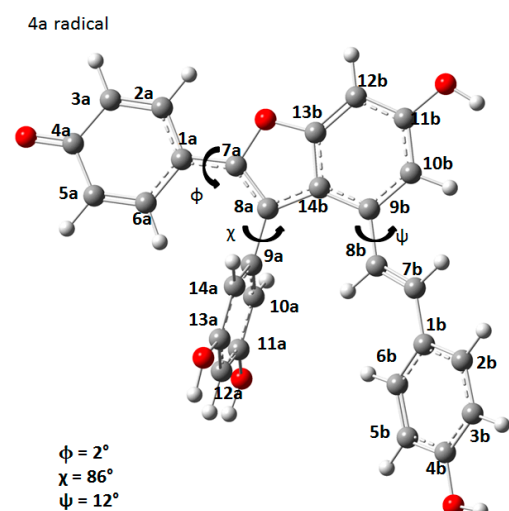


Bond type	Distance (Å)	Bond type	Distance (Å)	Bond type	Distance (Å)
1a-2a	1.406	1b-2b	1.431	H6a-H14a	3.360
2a-3a	1.389	2b-3b	1.364	H8b-H14a	3.333
3a-4a	1.396	3b-4b	1.456	H6a-H10a	3.256
4a-5a	1.396	4b-5b	1.461	H8b-H10a	3.218
5a-6a	1.386	5b-6b	1.361		
6a-1a	1.408	6b-1b	1.434		
1a-7a	1.458	1b-7b	1.426		
7a-8a	1.376	7b-8b	1.370		
8a-9a	1.487	8b-9b	1.445		
9a-10a	1.398	9b-10b	1.412		
10a-11a	1.394	10b-11b	1.393		
11a-12a	1.397	11b-12b	1.399		
12a-13a	1.397	12b-13b	1.380		
13a-14a	1.395	13b-14b	1.407		
14a-9a	1.398	14b-9b	1.424		
8a-14b	1.448				

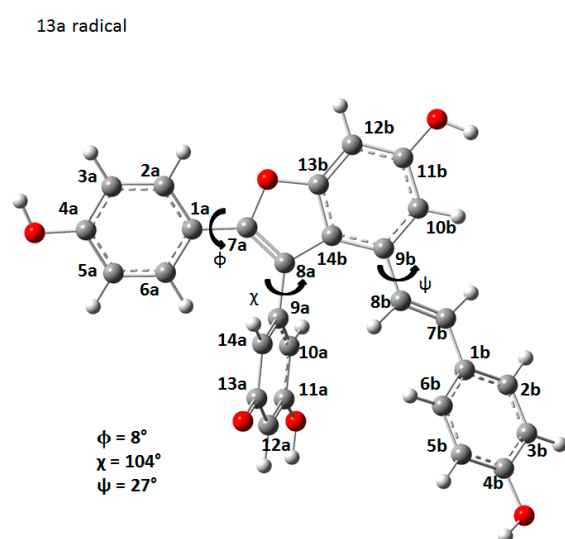


Bond type	Distance (Å)	Bond type	Distance (Å)	Bond type	Distance (Å)
1a-2a	1.409	1b-2b	1.406	H6a-H14a	3.253
2a-3a	1.387	2b-3b	1.389	H8b-H14a	3.230
3a-4a	1.397	3b-4b	1.394	H6a-H10a	3.350
4a-5a	1.397	4b-5b	1.398	H8b-H10a	3.542
5a-6a	1.384	5b-6b	1.389		
6a-1a	1.410	6b-1b	1.405		
1a-7a	1.451	1b-7b	1.464		
7a-8a	1.393	7b-8b	1.346		
8a-9a	1.487	8b-9b	1.468		
9a-10a	1.397	9b-10b	1.377		
10a-11a	1.394	10b-11b	1.461		
11a-12a	1.397	11b-12b	1.454		
12a-13a	1.396	12b-13b	1.361		
13a-14a	1.394	13b-14b	1.421		
14a-9a	1.398	14b-9b	1.442		
8a-14b	1.423				

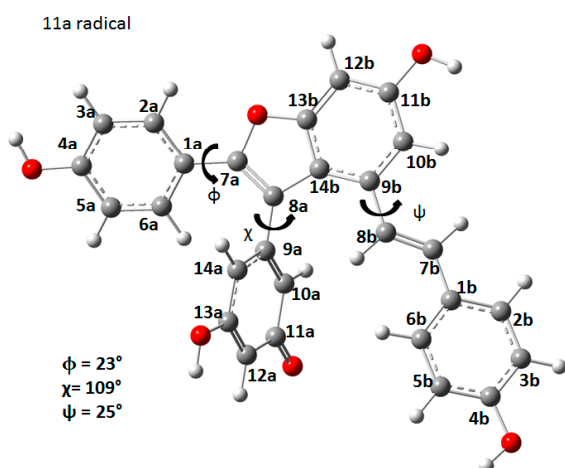
Figure S1. Optimized geometries of radical species of Vam3 and relative geometrical parameters.



Bond type	Distance (Å)	Bond type	Distance (Å)	Bond type	Distance (Å)
1a-2a	1.431	1b-2b	1.404	H6a-H14a	3.334
2a-3a	1.364	2b-3b	1.391	H8b-H14a	3.488
3a-4a	1.457	3b-4b	1.394	H6a-H10a	3.228
4a-5a	1.457	4b-5b	1.396	H8b-H10a	3.194
5a-6a	1.364	5b-6b	1.384		
6a-1a	1.430	6b-1b	1.409		
1a-7a	1.429	1b-7b	1.461		
7a-8a	1.393	7b-8b	1.348		
8a-9a	1.486	8b-9b	1.461		
9a-10a	1.398	9b-10b	1.401		
10a-11a	1.394	10b-11b	1.402		
11a-12a	1.397	11b-12b	1.396		
12a-13a	1.397	12b-13b	1.379		
13a-14a	1.394	13b-14b	1.411		
14a-9a	1.397	14b-9b	1.424		
8a-14b	1.437				



Bond type	Distance (Å)	Bond type	Distance (Å)	Bond type	Distance (Å)
1a-2a	1.405	1b-2b	1.406	H6a-H14a	3.401
2a-3a	1.390	2b-3b	1.388	H8b-H14a	3.495
3a-4a	1.397	3b-4b	1.395	H6a-H10a	3.379
4a-5a	1.396	4b-5b	1.398	H8b-H10a	3.308
5a-6a	1.386	5b-6b	1.388		
6a-1a	1.407	6b-1b	1.405		
1a-7a	1.460	1b-7b	1.463		
7a-8a	1.372	7b-8b	1.347		
8a-9a	1.484	8b-9b	1.465		
9a-10a	1.410	9b-10b	1.403		
10a-11a	1.417	10b-11b	1.401		
11a-12a	1.372	11b-12b	1.393		
12a-13a	1.449	12b-13b	1.373		
13a-14a	1.455	13b-14b	1.405		
14a-9a	1.383	14b-9b	1.417		
8a-14b	1.452				



Bond type	Distance (Å)	Bond type	Distance (Å)	Bond type	Distance (Å)
1a-2a	1.404	1b-2b	1.407	H6a-H14a	3.428
2a-3a	1.389	2b-3b	1.388	H8b-H14a	3.750
3a-4a	1.396	3b-4b	1.394	H6a-H10a	3.339
4a-5a	1.396	4b-5b	1.398	H8b-H10a	3.062
5a-6a	1.387	5b-6b	1.387		
6a-1a	1.406	6b-1b	1.405		
1a-7a	1.460	1b-7b	1.462		
7a-8a	1.372	7b-8b	1.347		
8a-9a	1.484	8b-9b	1.465		
9a-10a	1.385	9b-10b	1.403		
10a-11a	1.454	10b-11b	1.400		
11a-12a	1.449	11b-12b	1.392		
12a-13a	1.372	12b-13b	1.382		
13a-14a	1.417	13b-14b	1.406		
14a-9a	1.408	14b-9b	1.418		
8a-14b	1.454				

Figure S2. Optimized geometries of radical species of Vam3 and relative geometrical parameters.

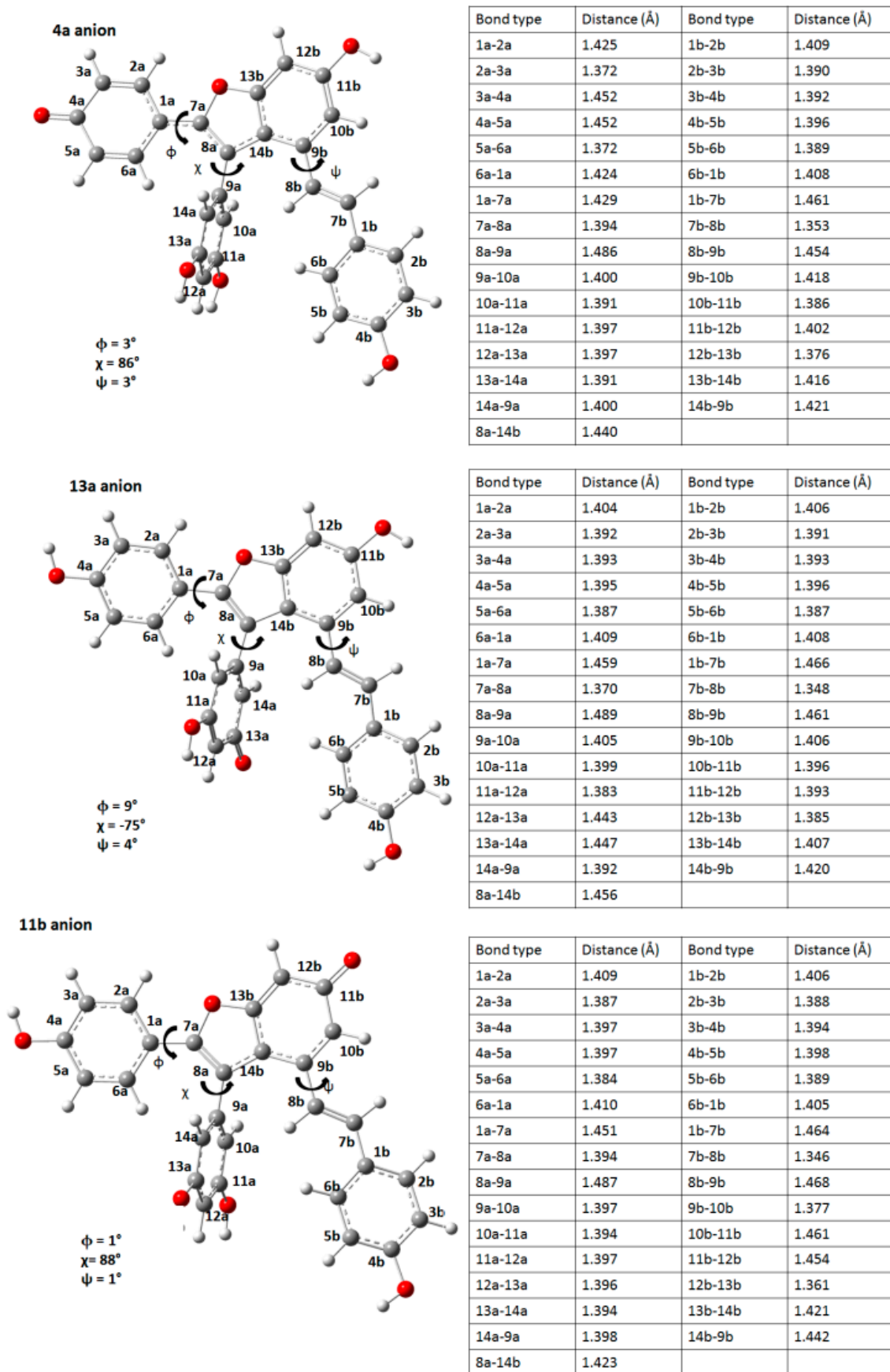
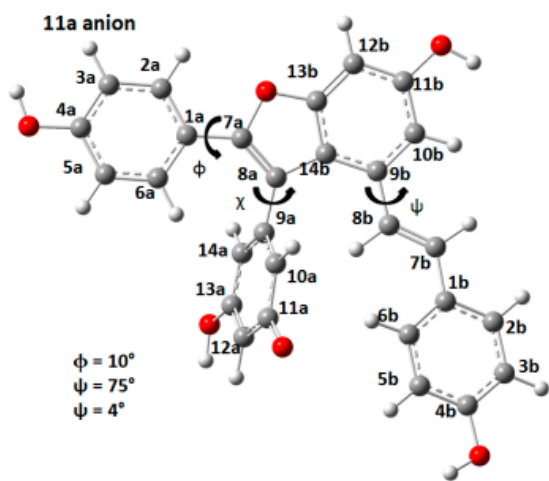
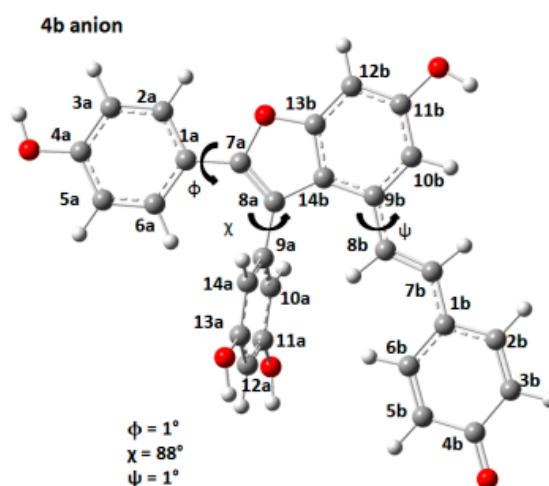


Figure S3. Optimized geometries of anion species of Vam3 and relative geometrical parameters.



Bond type	Distance (Å)	Bond type	Distance (Å)
1a-2a	1.404	1b-2b	1.406
2a-3a	1.392	2b-3b	1.391
3a-4a	1.393	3b-4b	1.393
4a-5a	1.395	4b-5b	1.396
5a-6a	1.387	5b-6b	1.387
6a-1a	1.409	6b-1b	1.408
1a-7a	1.459	1b-7b	1.466
7a-8a	1.370	7b-8b	1.348
8a-9a	1.489	8b-9b	1.461
9a-10a	1.391	9b-10b	1.406
10a-11a	1.447	10b-11b	1.396
11a-12a	1.443	11b-12b	1.393
12a-13a	1.383	12b-13b	1.385
13a-14a	1.399	13b-14b	1.407
14a-9a	1.405	14b-9b	1.420
8a-14b	1.456		



Bond type	Distance (Å)	Bond type	Distance (Å)
1a-2a	1.407	1b-2b	1.424
2a-3a	1.391	2b-3b	1.373
3a-4a	1.393	3b-4b	1.451
4a-5a	1.394	4b-5b	1.456
5a-6a	1.388	5b-6b	1.370
6a-1a	1.409	6b-1b	1.425
1a-7a	1.457	1b-7b	1.427
7a-8a	1.373	7b-8b	1.371
8a-9a	1.487	8b-9b	1.441
9a-10a	1.398	9b-10b	1.406
10a-11a	1.392	10b-11b	1.396
11a-12a	1.396	11b-12b	1.396
12a-13a	1.396	12b-13b	1.386
13a-14a	1.392	13b-14b	1.404
14a-9a	1.398	14b-9b	1.433
8a-14b	1.451		

**Figure S4.** Optimized geometries of anion species of Vam3 and relative geometrical parameters.

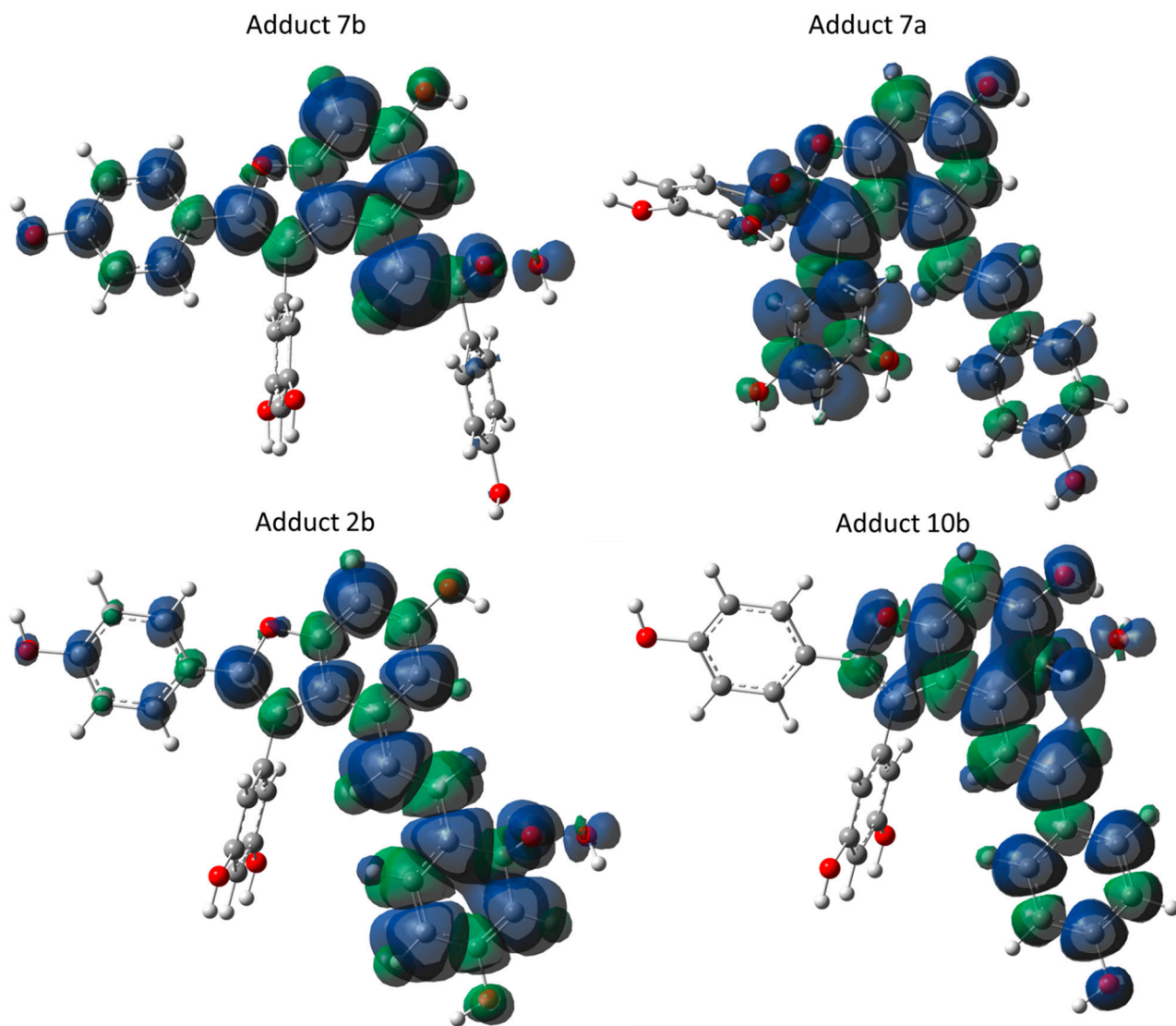


Figure S5. Spin densities of adducts obtained by exergonic radical adduct formation mechanism.

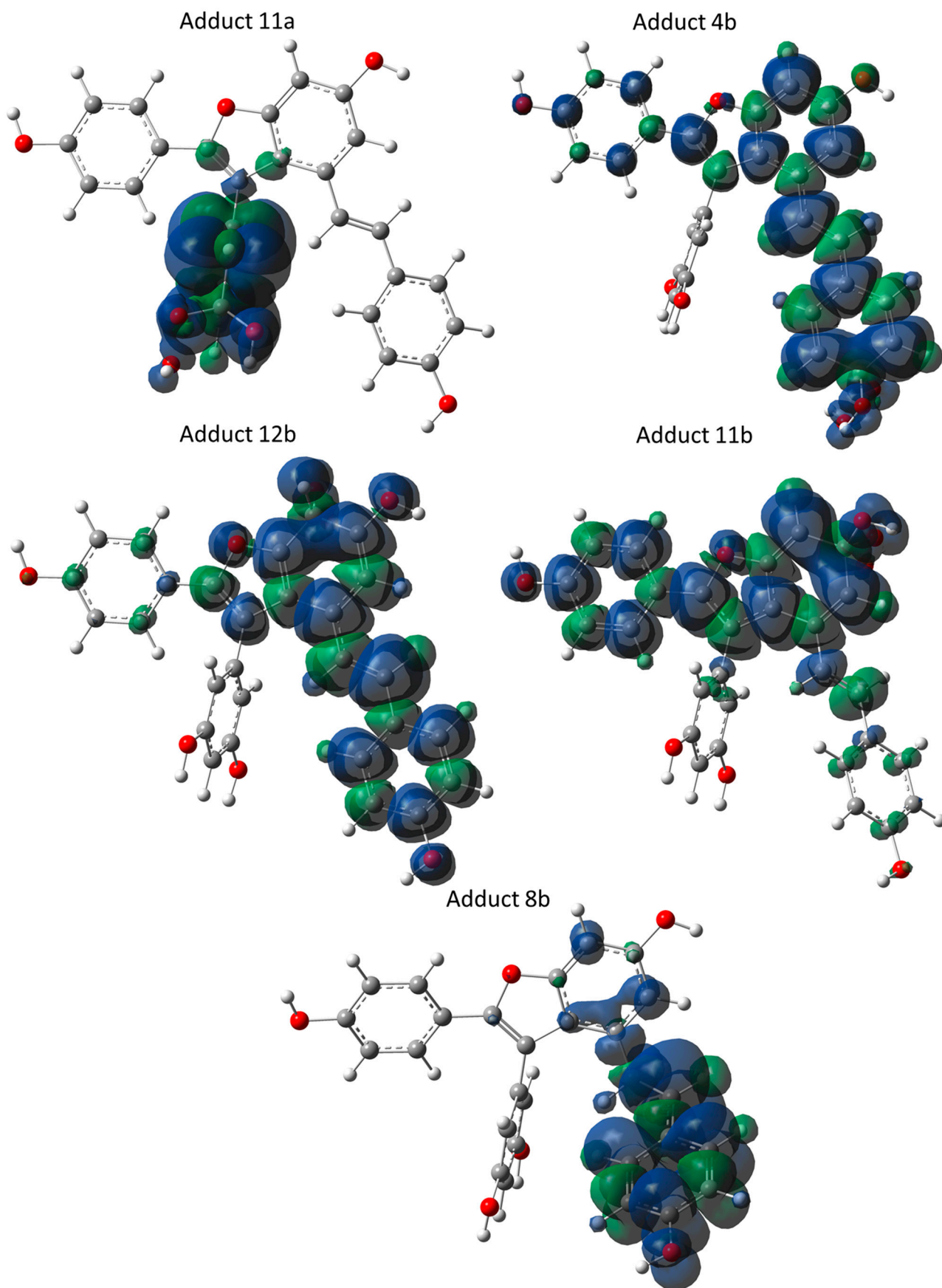
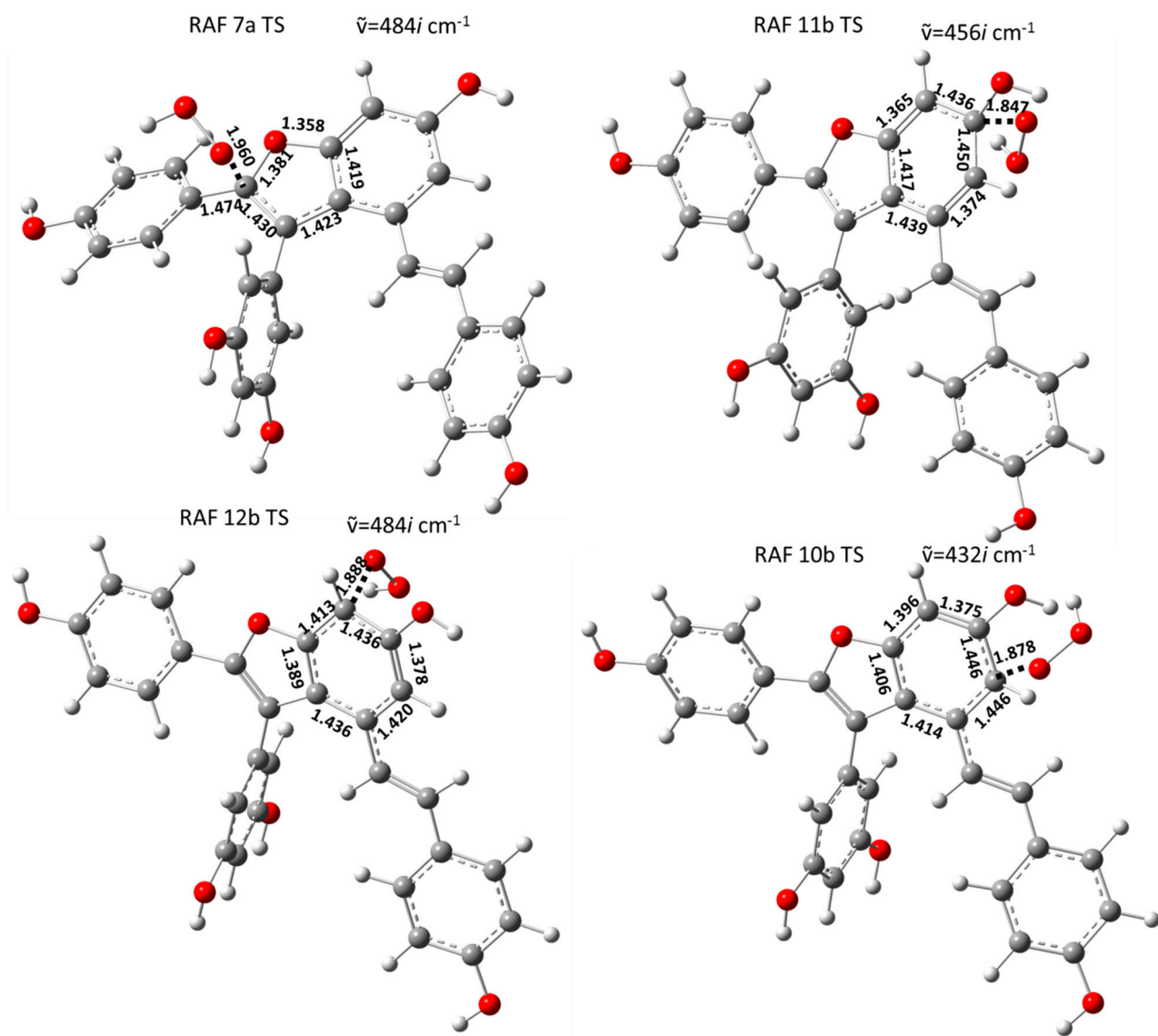
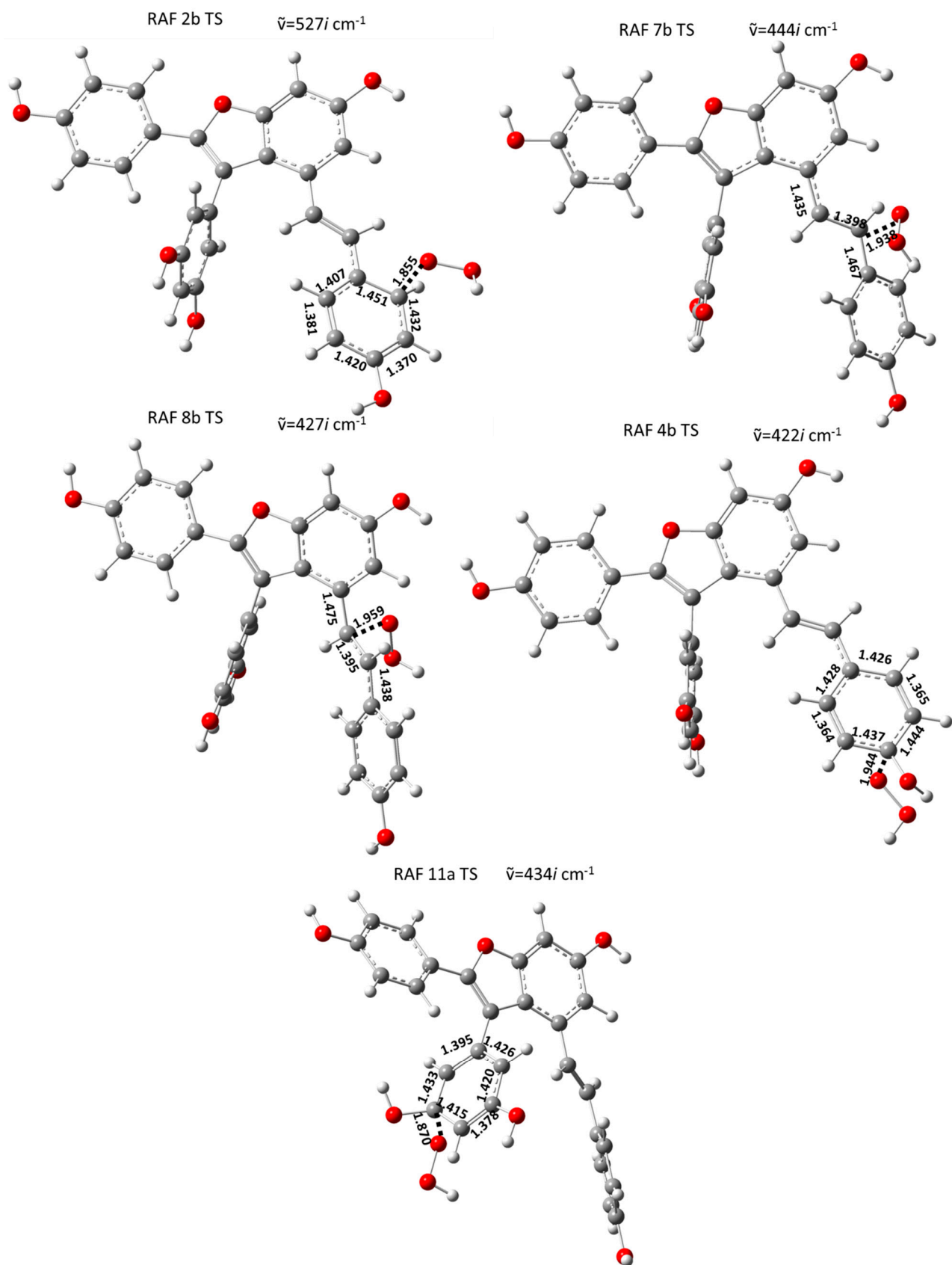


Figure S6. Spin densities of adducts obtained by exergonic radical adduct formation mechanism.



**Figure S5.** Optimized geometries of RAF Transition State species of Vam3 and relative geometrical parameters.





**Figure S6.** Optimized geometries of RAF Transition State species of Vam3 and relative geometrical parameters.

## Cartesian coordinates 4a HAT TS

C	0.90937200	2.82240100	0.08728100
C	-0.08071600	1.81789800	0.11529000
C	-1.44859700	2.20995700	0.15174100
C	-1.70530900	3.58807000	0.16921500
C	-0.68423400	4.54641100	0.13465400
C	0.66238900	4.17923400	0.09217100
C	1.98700700	0.88929800	0.03973000
C	0.63644800	0.57090200	0.07977700
H	-2.73105300	3.93261300	0.24797900
H	1.44969300	4.92005900	0.07407700
C	3.20745600	0.12935200	-0.01186000
C	4.45655300	0.80163600	-0.01050900
C	3.22148100	-1.28887900	-0.07108800
C	5.64763900	0.11459800	-0.06092500
H	4.46961900	1.88246600	0.03242700
C	4.40438400	-1.98429800	-0.12397000
H	2.29056900	-1.83654500	-0.07813600
C	5.65551700	-1.30774400	-0.11921000
H	6.59179600	0.64491000	-0.05795100
H	4.41571200	-3.06644900	-0.17135400
C	0.04545800	-0.79275200	0.08182200
C	-0.13739600	-1.47179400	1.29041300
C	-0.34053300	-1.38079600	-1.12511900
C	-0.70214800	-2.74672600	1.28168900
H	0.15957700	-1.02963000	2.23255100
C	-0.90477500	-2.65585400	-1.11837900
H	-0.20786600	-0.86532400	-2.06724800
C	-1.08796300	-3.34727300	0.08131200
H	-1.52499000	-4.34265200	0.08042100
C	-2.52671800	1.22465900	0.18488300
H	-2.24142500	0.23218700	0.50934000
C	-3.80736200	1.44875300	-0.17406800
H	-4.07320900	2.42457200	-0.57363600
C	-4.91419500	0.49651600	-0.12294500
C	-4.81879500	-0.77834200	0.46975100
C	-6.15085700	0.85405900	-0.68363200
C	-5.89487500	-1.64914200	0.49011400
H	-3.88965000	-1.09228500	0.93004000

C	-7.23936600	-0.01158100	-0.66963200
H	-6.26150800	1.83034500	-1.14410300
C	-7.11350800	-1.27028400	-0.08254200
H	-5.81650600	-2.62556400	0.95292400
H	-8.18291900	0.29238800	-1.11319100
O	6.74662300	-2.01717800	-0.16764100
O	-1.25991200	-3.18582100	-2.32530200
O	-0.85703200	-3.36821500	2.48879200
O	-0.95396200	5.88522600	0.15878300
O	-8.13884900	-2.17230300	-0.02955000
O	2.14624100	2.26480000	0.04639100
H	-1.90591200	6.02721500	0.19099600
H	-8.92503800	-1.80076600	-0.44361900
H	-1.64996000	-4.05799900	-2.20560000
H	-1.22607600	-4.24902400	2.36541900
H	7.72623100	-1.48726900	-0.18085300
O	8.95065000	-1.05340400	-0.21636300
O	8.87496900	0.34815600	-0.15653800
H	9.80494300	0.60697000	-0.22484200

## Cartesian coordinates 11b HAT TS

C	1.31651300	2.60537400	-0.12855200
C	0.51540600	1.43970600	-0.14344700
C	-0.90828100	1.58835600	-0.21331700
C	-1.40162400	2.88588500	-0.27227000
C	-0.56683200	4.03944700	-0.22604200
C	0.84271500	3.89040900	-0.15235300
C	2.70617300	0.88832100	-0.03075200
C	1.43125700	0.34082900	-0.07587900
H	-2.46422900	3.05671300	-0.38833200
H	1.48512300	4.75982200	-0.12207600
C	4.04948100	0.34434800	0.05259400
C	5.15664100	1.21323100	-0.00643400
C	4.30420200	-1.03472300	0.20008600
C	6.45401900	0.72951900	0.07231700
H	4.99267100	2.27661100	-0.11594200
C	5.59801600	-1.52061700	0.28065800
H	3.48292800	-1.73376500	0.25712500
C	6.68219700	-0.64144300	0.21571800

H	7.29155500	1.41896600	0.02251600
H	5.78773100	-2.58062000	0.39623200
C	1.09129500	-1.10626900	-0.04791300
C	0.75554300	-1.71343600	1.16460800
C	1.09864900	-1.84858600	-1.23265200
C	0.43056400	-3.06904000	1.18719700
H	0.73891600	-1.14957000	2.08801000
C	0.77367300	-3.20383200	-1.19450800
H	1.35611400	-1.39133500	-2.17921800
C	0.43964100	-3.82322900	0.01162400
H	0.18906300	-4.88079500	0.03576700
C	-1.79448600	0.42464900	-0.25190400
H	-1.34961000	-0.49981600	-0.59924700
C	-3.08768400	0.42847600	0.12878500
H	-3.49777500	1.33998800	0.55634000
C	-4.02642600	-0.68993100	0.06372500
C	-3.76758500	-1.88183100	-0.63498500
C	-5.26719000	-0.58194500	0.71845700
C	-4.69380000	-2.91545600	-0.66526600
H	-2.83686000	-2.00109500	-1.17682200
C	-6.20053900	-1.60863700	0.69731800
H	-5.49976500	0.33029400	1.25773200
C	-5.91504000	-2.78403200	0.00325300
H	-4.47599300	-3.82335200	-1.22097700
H	-7.15212700	-1.51377100	1.20598700
O	7.93268500	-1.17780100	0.29902400
O	0.79843900	-3.88532700	-2.37956900
O	0.11450800	-3.61370900	2.39860200
O	-1.06207800	5.24987500	-0.28287900
O	-6.86541100	-3.76785000	0.00295800
O	2.63639500	2.26205700	-0.06668300
H	8.59536200	-0.48048100	0.24700700
H	-0.13612300	-4.53750200	2.29464100
H	-2.12704700	5.29847700	0.01578100
H	0.57333000	-4.81038100	-2.23587200
H	-6.56618800	-4.51098700	-0.53120400
O	-3.31904400	5.36190000	0.54491400
O	-3.97763100	6.35762600	-0.19178100
H	-4.54896800	6.76518400	0.47547700

Cartesian coordinates 13a HAT TS

C	1.07214900	3.13820300	-0.10297400
C	0.16142500	2.06883200	-0.05862400
C	-1.21908600	2.34658400	-0.21874400
C	-1.57803700	3.69291500	-0.38029000
C	-0.63443600	4.72834600	-0.38783800
C	0.72807400	4.46906300	-0.25661300
C	2.27778700	1.30827600	0.18738600
C	0.97470800	0.88257500	0.13837400
H	-2.62020600	3.94086600	-0.55389600
H	1.46021800	5.26429900	-0.28649300
C	3.56544800	0.64003500	0.35529500
C	4.73755600	1.24499000	-0.12689500
C	3.68558300	-0.60291200	1.00065600
C	5.97469700	0.62611200	0.00697800
H	4.67546000	2.20774600	-0.61749300
C	4.91803400	-1.22865200	1.13590700
H	2.80946200	-1.08147600	1.41669300
C	6.07059900	-0.61695800	0.63509600
H	6.86615700	1.11160000	-0.37895800
H	5.00765700	-2.17701800	1.65268400
C	0.51763900	-0.52372500	0.25320700
C	-0.19405300	-0.93857100	1.38499500
C	0.79815900	-1.44272000	-0.75719400
C	-0.61071000	-2.27771000	1.51153400
H	-0.43726600	-0.24088400	2.17646000
C	0.41610500	-2.80513600	-0.61477400
H	1.31942400	-1.13778700	-1.65329400
C	-0.30179600	-3.20843400	0.53718900
H	-0.58406200	-4.25165800	0.62861900
C	-2.22128500	1.27885800	-0.25730600
H	-1.85558300	0.30715500	-0.56745900
C	-3.52260500	1.40927800	0.06501900
H	-3.86664900	2.36238600	0.46053500
C	-4.55450400	0.37500900	-0.02031400
C	-4.37951800	-0.83633700	-0.71105200
C	-5.79513000	0.58483800	0.60810900
C	-5.38349500	-1.79426200	-0.75512500
H	-3.45264800	-1.03211100	-1.23690800

C	-6.80693600	-0.36472900	0.57213000
H	-5.96506100	1.51373600	1.14286100
C	-6.60240600	-1.56365100	-0.11043900
H	-5.22527700	-2.71892600	-1.30290900
H	-7.75727700	-0.19232300	1.06254300
O	7.25522400	-1.27749400	0.79799200
O	0.70020400	-3.69840900	-1.53118500
O	-1.30034500	-2.58712400	2.64631100
O	-1.00231800	6.03768200	-0.55361200
O	-7.62787400	-2.46859600	-0.12441000
O	2.34729600	2.68142700	0.03535300
H	-1.95970800	6.09790500	-0.63482600
H	-7.37492700	-3.24142300	-0.64027500
H	-1.55178400	-3.51723200	2.63613300
H	7.97699300	-0.75385300	0.43382500
H	1.77359600	-3.67094800	-1.95387600
O	2.98626500	-3.73912300	-2.12706800
O	3.40326900	-2.42723400	-1.93375300
H	4.10391900	-2.49980500	-1.26315800

Cartesian coordinates 11a HAT TS

C	1.66798200	2.91260100	0.31559300
C	0.65396900	1.94517200	0.18366800
C	-0.69905300	2.37845600	0.23254100
C	-0.91713600	3.74666800	0.46537600
C	0.12824700	4.66407300	0.60577000
C	1.46204200	4.26172900	0.52454500
C	2.69534300	0.98770400	-0.02385100
C	1.35073600	0.69383100	-0.04586900
H	-1.93589400	4.10532100	0.56820700
H	2.27339200	4.96923900	0.62667600
C	3.90869100	0.19764200	-0.17395600
C	5.11761700	0.83019900	-0.51412300
C	3.92733200	-1.19574800	0.02979600
C	6.28942000	0.10200000	-0.66419100
H	5.13332700	1.90162900	-0.66518100
C	5.09549600	-1.92670100	-0.11808400
H	3.02470800	-1.71033600	0.32785600
C	6.28270700	-1.28188200	-0.47042600
H	7.21120000	0.60956300	-0.93287500

H	5.10697400	-2.99691000	0.04765300
C	0.76859400	-0.64612700	-0.30653500
C	0.09780600	-1.34682900	0.69149200
C	0.85870400	-1.18824700	-1.59782600
C	-0.49116500	-2.61146500	0.41072100
H	0.01381600	-0.94390400	1.69348000
C	0.27214600	-2.43378400	-1.88290100
H	1.36439200	-0.65278300	-2.39089200
C	-0.38588400	-3.14668600	-0.89865100
H	-0.83316300	-4.11537700	-1.09420400
C	-1.81068000	1.44977000	0.05215400
H	-1.57935000	0.40503900	0.21285600
C	-3.06596100	1.77935600	-0.31959100
H	-3.28138200	2.81364900	-0.57763100
C	-4.20018900	0.87017400	-0.45762600
C	-4.18872500	-0.45815500	0.00604900
C	-5.37860600	1.32804600	-1.07632100
C	-5.28849600	-1.28746100	-0.15684600
H	-3.31764000	-0.85175200	0.51529500
C	-6.48525800	0.50851500	-1.24481600
H	-5.42149300	2.35046800	-1.43761000
C	-6.44228900	-0.80846800	-0.78575600
H	-5.25453100	-2.30700100	0.21606600
H	-7.38595300	0.87087400	-1.72515700
O	7.40232900	-2.05108300	-0.60347000
O	0.40195700	-2.88267500	-3.16539800
O	-1.14035200	-3.28885700	1.31949000
O	-0.10110300	5.99357000	0.83737700
O	-7.55546000	-1.57952200	-0.96840100
O	2.89518700	2.33592100	0.19167800
H	-1.04897100	6.15725600	0.87998400
H	-7.40808100	-2.45794400	-0.60183800
H	8.15642500	-1.49744600	-0.83276500
H	-0.03446200	-3.73641500	-3.25941100
O	-0.40003800	-2.84329200	3.54034800
O	-1.52093000	-2.99108100	4.36952700
H	-1.13587500	-3.38866700	5.16445700
H	-0.84049900	-3.01466400	2.41381200

### Cartesian coordinates 4b HAT TS

C	-2.63301112	2.78884232	-0.10757714
C	-1.44563412	2.03912832	-0.03908714
C	-0.21000512	2.73107132	0.03440086
C	-0.27104312	4.13411732	0.02831886
C	-1.47860812	4.83516632	-0.05539014
C	-2.70150812	4.16967532	-0.12365414
C	-3.23914412	0.66164032	-0.13221314
C	-1.86947412	0.65026132	-0.05932314
H	0.64821188	4.70203332	0.12783586
H	-3.63701412	4.70967632	-0.17482214
C	-4.27350512	-0.36707668	-0.17882314
C	-5.60994812	-0.02814868	0.09017786
C	-3.98763312	-1.70719768	-0.49762214
C	-6.61578612	-0.98646268	0.05613186
H	-5.86071312	0.99643132	0.33110186
C	-4.98782812	-2.66701968	-0.53331114
H	-2.97424212	-2.00245368	-0.73109714
C	-6.30833212	-2.31183668	-0.25334714
H	-7.64129912	-0.70078368	0.27203186
H	-4.76175412	-3.69632968	-0.78387914
C	-1.00119212	-0.55342868	0.01647586
C	-0.31905912	-0.99733668	-1.12113314
C	-0.85773312	-1.23094368	1.23078886
C	0.50105888	-2.12056268	-1.03758614
H	-0.41446912	-0.48010168	-2.06696114
C	-0.03554512	-2.35460168	1.29960886
H	-1.37712012	-0.89838168	2.11996586
C	0.64867688	-2.80768668	0.16988986
H	1.28665088	-3.68617068	0.22836386
C	1.06146288	2.01421232	0.13254286
H	0.98566188	0.98201532	0.44964086
C	2.28020388	2.51602632	-0.14992614
H	2.35157988	3.53412032	-0.52536814
C	3.56407388	1.82553532	-0.03721914
C	3.70451288	0.51815232	0.46260686
C	4.73663988	2.48460832	-0.44891114
C	4.94530788	-0.09702668	0.54137986
H	2.83260788	-0.03134468	0.79676786

C	5.98459588	1.88092932	-0.37604914
H	4.66381388	3.49528532	-0.83768114
C	6.09500088	0.58247732	0.12235386
H	5.02951988	-1.10804768	0.92747386
H	6.87950188	2.40067932	-0.69651314
O	-7.25343912	-3.29985368	-0.30221214
O	0.06766088	-2.98156168	2.51091986
O	1.13966788	-2.51656868	-2.18006814
O	-1.51931012	6.20619932	-0.05378614
O	7.34122688	0.02868632	0.18489486
O	-3.71254612	1.96307732	-0.15982414
H	-8.11945912	-2.93221868	-0.09686514
H	1.70512888	-3.27400768	-1.99733914
H	-0.62356712	6.55499032	-0.00289514
H	0.66253688	-3.73552668	2.44343986
H	7.27743600	-1.03146500	0.56190800
O	7.27821120	-2.14334304	0.37790905
O	6.84915220	-2.63813604	-0.77609695
H	7.63375620	-2.67117604	-1.35854895

### Cartesian coordinates 4b radical

C	1.53527338	2.77794243	0.00895209
C	0.53282698	1.79056700	0.01324689
C	-0.82829522	2.20834292	0.00648401
C	-1.06466705	3.60059609	0.00471391
C	-0.03241687	4.53613542	0.00550821
C	1.30919033	4.13906728	0.00607601
C	2.58275434	0.83090618	0.01383375
C	1.24086297	0.52759924	0.01718397
H	-2.08539917	3.96606706	-0.00110281
H	2.11014931	4.86574353	0.00356295
C	3.81537537	0.05189588	0.01041580
C	5.05430843	0.70689190	-0.10259001
C	3.82386920	-1.35181027	0.12052224
C	6.24656541	-0.00515895	-0.11006516
H	5.08149438	1.78486194	-0.18655826
C	5.01121859	-2.06626941	0.11415200
H	2.89434131	-1.89354119	0.21693780
C	6.23097426	-1.39676811	-0.00227017
H	7.19061551	0.52409821	-0.20037402

H	5.01032851	-3.14592117	0.20065713
C	0.63936306	-0.83266887	0.01663786
C	0.29373094	-1.44152116	1.22710436
C	0.40143227	-1.48775432	-1.19498330
C	-0.28634098	-2.70974206	1.21867192
H	0.46996390	-0.94617210	2.17312935
C	-0.17888996	-2.75617419	-1.18917611
H	0.66114823	-1.02858987	-2.13989913
C	-0.52666419	-3.37500518	0.01386603
H	-0.97442117	-4.36560541	0.01291722
C	-1.90226732	1.24100214	-0.00345182
H	-1.58916796	0.20667600	-0.01478574
C	-3.24711045	1.50378998	-0.00032915
H	-3.57924114	2.53804045	0.01494026
C	-4.29850309	0.54025610	-0.01400679
C	-4.07469339	-0.87583333	-0.03738002
C	-5.65499922	0.99527392	-0.00412917
C	-5.11058855	-1.75821311	-0.04981304
H	-3.05850638	-1.25206195	-0.04531186
C	-6.70906262	0.13014215	-0.01600708
H	-5.83470253	2.06622231	0.01355805
C	-6.50220353	-1.31347085	-0.03959410
H	-4.94388555	-2.82933824	-0.06783894
H	-7.73486161	0.48008389	-0.00829009
O	7.36785655	-2.15309999	-0.00338515
O	-0.38405409	-3.35240032	-2.40015909
O	-0.59861113	-3.25992024	2.42865898
O	-0.26743824	5.88467961	0.00326714
O	-7.44888946	-2.11776418	-0.05034381
O	2.76582903	2.20209598	0.00807313
H	-1.21549527	6.05259126	0.00344600
H	8.14075273	-1.58483188	-0.08928120
H	-0.81091704	-4.20780846	-2.28433541
H	-1.01600286	-4.11936442	2.30828704

### Cartesian coordinates 4a radical

C	1.68128714	2.73996496	0.06402304
C	0.66085084	1.76603911	0.10095591
C	-0.69452503	2.19916328	0.15312326
C	-0.90871905	3.58352642	0.17619327

C 0.14121095 4.51123340 0.13154076  
C 1.47498527 4.10422730 0.07378001  
C 2.70101434 0.77423130 0.00106894  
C 1.33669591 0.49851725 0.05478890  
H -1.92267610 3.95816539 0.26827011  
H 2.28409623 4.82089734 0.04845094  
C 3.88789753 -0.01934990 -0.06374205  
C 5.16611459 0.62308716 -0.08468000  
C 3.85206112 -1.44761093 -0.11352598  
C 6.32281245 -0.09767077 -0.14721923  
H 5.20256114 1.70394704 -0.04884782  
C 4.99999738 -2.18185918 -0.17801576  
H 2.89818737 -1.95478817 -0.10214920  
C 6.31426729 -1.55360990 -0.19792076  
H 7.29118564 0.38916806 -0.16160015  
H 4.97342528 -3.26473734 -0.21752413  
C 0.70097888 -0.84472511 0.05840582  
C 0.50138327 -1.51799733 1.26745201  
C 0.29000395 -1.41743725 -1.14739016  
C -0.10519991 -2.77362646 1.25990012  
H 0.81743227 -1.08733595 2.20871334  
C -0.31601724 -2.67334102 -1.13920114  
H 0.43547001 -0.90583027 -2.08971725  
C -0.51594517 -3.35968550 0.06066118  
H -0.98553389 -4.34009430 0.06096916  
C -1.80335933 1.24812011 0.19763924  
H -1.55021734 0.25086918 0.53398694  
C -3.07561416 1.51029992 -0.16409628  
H -3.30847120 2.48958898 -0.57573321  
C -4.21416758 0.59647907 -0.10084690  
C -4.16117948 -0.67309124 0.50798793  
C -5.43853239 0.98862111 -0.66497313  
C -5.26628361 -1.50642793 0.54081915  
H -3.24270399 -1.01246425 0.97165833  
C -6.55597853 0.16083284 -0.63858729  
H -5.51652465 1.96207811 -1.13796234  
C -6.47215367 -1.09372894 -0.03541625  
H -5.22068335 -2.47876995 1.01642408  
H -7.48923341 0.49109501 -1.08508324

O 7.36409463 -2.21930800 -0.25512376  
O -0.69427208 -3.18929730 -2.34477116  
O -0.27484408 -3.39079636 2.46693808  
O -0.08868005 5.85680256 0.16079527  
O -7.52736063 -1.95963913 0.03042187  
O 2.89988815 2.14740816 0.00903623  
H -1.03553108 6.02738549 0.20359089  
H -8.30107650 -1.56746217 -0.38809383  
H -1.11287087 -4.04810912 -2.22471301  
H -0.67075492 -4.26002926 2.34462934

### Cartesian coordinates 11a radical

C 1.61229301 2.75408712 -0.04122185  
C 0.60351025 1.77708410 -0.07399485  
C -0.74782006 2.19809328 -0.13254091  
C -0.97907316 3.58189920 -0.13290022  
C 0.06049078 4.51889853 -0.07624227  
C 1.39490223 4.12005023 -0.03565279  
C 2.64328005 0.79565715 0.00156478  
C 1.30296086 0.50540819 -0.04053286  
H -1.99816906 3.94268854 -0.22744091  
H 2.19989037 4.84172312 -0.01220706  
C 3.86826611 0.00316395 0.05420574  
C 5.09688021 0.59455181 -0.28301828  
C 3.87645936 -1.34655501 0.44978584  
C 6.28000941 -0.13262822 -0.24110691  
H 5.12281731 1.63368817 -0.58344385  
C 5.05387133 -2.07724296 0.49335618  
H 2.95517447 -1.83233232 0.73946594  
C 6.26360439 -1.47377504 0.14465695  
H 7.21723577 0.34566017 -0.51021630  
H 5.05357023 -3.11526699 0.80256715  
C 0.68472890 -0.84401231 -0.04605906  
C 0.05825501 -1.32048986 1.12389098  
C 0.69080703 -1.63942710 -1.17700821  
C -0.55447086 -2.59720194 1.15980995  
H 0.03548874 -0.71319917 2.02042202  
C 0.06678217 -2.95340226 -1.17901009  
H 1.15500184 -1.31054185 -2.09857833  
C -0.55728820 -3.40277746 0.04855307

H -1.01758986 -4.38510453 0.04496419  
C -1.85344331 1.24117889 -0.22694190  
H -1.60800403 0.28380993 -0.67150900  
C -3.11586444 1.45627303 0.19118909  
H -3.33728701 2.38317302 0.71561486  
C -4.25317959 0.54595428 0.05120795  
C -4.24528532 -0.57666614 -0.79415905  
C -5.42815523 0.79256729 0.78394699  
C -5.34528131 -1.41862525 -0.88732229  
H -3.37583123 -0.79054795 -1.40434223  
C -6.53462464 -0.04115094 0.70023485  
H -5.46960462 1.65641528 1.43942721  
C -6.49550256 -1.15577391 -0.13730509  
H -5.31570824 -2.27529442 -1.55463121  
H -7.43293583 0.15781812 1.27191932  
O 7.39212250 -2.24141808 0.20603410  
O 0.06455592 -3.66255110 -2.20978492  
O -1.11600783 -2.94183709 2.35357138  
O -0.18261695 5.86739033 -0.08553515  
O -7.60951275 -1.94705001 -0.19232788  
O 2.83885920 2.16558804 -0.00459802  
H -1.13171328 6.02568154 -0.11607503  
H -7.46737944 -2.66944945 -0.81310519  
H -1.52536930 -3.81178120 2.28716440  
H 8.15850663 -1.71893810 -0.05318178

### Cartesian coordinates 13a radical

C -1.49634128 2.80123522 0.04931297  
C -0.51599491 1.79360607 0.06851522  
C 0.84583321 2.17812637 0.15859230  
C 1.11069224 3.55537525 0.21040987  
C 0.09866827 4.52160739 0.16793228  
C -1.24422007 4.16037248 0.09020197  
C -2.58531027 0.88088327 -0.06222701  
C -1.25642713 0.54473030 -0.00610618  
H 2.13672724 3.88833727 0.32770889  
H -2.03045628 4.90253828 0.07385886  
C -3.82894348 0.12156313 -0.15441974  
C -5.03367528 0.69520608 0.28334584  
C -3.87587621 -1.17629594 -0.69406888

C -6.23171141 -0.00397783 0.20428994  
H -5.02884337 1.69807846 0.69038528  
C -5.06852425 -1.87937512 -0.77470279  
H -2.97451855 -1.63584510 -1.07612586  
C -6.25355955 -1.29711186 -0.32141221  
H -7.15082085 0.45825109 0.55239596  
H -5.10020239 -2.87549996 -1.19882724  
C -0.71774321 -0.83801409 0.01634681  
C 0.00061120 -1.35481388 -1.04907908  
C -0.94036226 -1.64872792 1.14632016  
C 0.51709402 -2.71358495 -1.02415483  
H 0.19698306 -0.76937080 -1.93885729  
C -0.45271325 -2.97842599 1.20433016  
H -1.49534325 -1.26686303 1.99426108  
C 0.25837979 -3.50965645 0.15846583  
H 0.64171314 -4.52444749 0.17221809  
C 1.92802503 1.19227391 0.21740083  
H 1.64706789 0.20914619 0.57444307  
C 3.20709036 1.41315091 -0.14420292  
H 3.46450810 2.38514897 -0.55841112  
C 4.32692150 0.47505194 -0.07810021  
C 4.22796852 -0.82456029 0.44764109  
C 5.58314542 0.87684406 -0.56713513  
C 5.32246318 -1.67674045 0.47691094  
H 3.28353795 -1.18318741 0.83893486  
C 6.68662445 0.03551996 -0.54176902  
H 5.69295023 1.87436592 -0.98012517  
C 6.55863023 -1.25059348 -0.01882178  
H 5.21807239 -2.67868148 0.88322699  
H 7.64778179 0.35680570 -0.92414086  
O -7.39859593 -2.03542102 -0.42446313  
O -0.74115613 -3.65581097 2.35317714  
O 1.15528389 -3.17715427 -1.99531309  
O 0.37790717 5.86193928 0.22514799  
O 7.66959130 -2.04732328 -0.01390572  
O -2.74054018 2.25335526 -0.02395215  
H 1.33060138 5.99279846 0.26989416  
H 7.44871536 -2.91420663 0.34247717  
H -8.14784053 -1.52595192 -0.09798511

### Cartesian coordinates 11b radical

C -1.64816646 2.80943324 0.08379786  
C -0.62320411 1.82514503 0.12098897  
C 0.75224292 2.25431625 0.18973809  
C 0.97668499 3.61233218 0.21316688  
C -0.07569933 4.62324012 0.14801670  
C -1.45128342 4.15661638 0.08893670  
C -2.65324022 0.83825380 0.00967019  
C -1.28719297 0.56758229 0.06646202  
H 1.98190109 4.00151241 0.31875097  
H -2.25816442 4.87640063 0.05322676  
C -3.85061646 0.02285622 -0.06516130  
C -5.11569564 0.63994781 -0.00397095  
C -3.80956448 -1.37961430 -0.20799788  
C -6.28228435 -0.10629001 -0.07452086  
H -5.17833753 1.71447608 0.10148297  
C -4.97250133 -2.12697398 -0.28096031  
H -2.85984425 -1.89038042 -0.26834790  
C -6.21716168 -1.49525699 -0.21278799  
H -7.24598544 0.39153084 -0.02254930  
H -4.93557164 -3.20352635 -0.39328083  
C -0.65550033 -0.77866527 0.05791369  
C -0.18646830 -1.31143087 -1.14481306  
C -0.52458187 -1.49763829 1.24984311  
C 0.41141785 -2.57101719 -1.15137010  
H -0.27297026 -0.76184484 -2.07290212  
C 0.07385198 -2.75664728 1.22772509  
H -0.88228188 -1.09660025 2.18937826  
C 0.54205319 -3.30287038 0.03095581  
H 1.00416516 -4.28683314 0.01980075  
C 1.85003806 1.28250022 0.25916191  
H 1.61548712 0.32950386 0.71881585  
C 3.09122224 1.49626296 -0.21548733  
H 3.28357023 2.42089119 -0.75467820  
C 4.23800702 0.59200699 -0.11843199  
C 4.27135947 -0.52777599 0.72941104  
C 5.38129341 0.84578611 -0.89711895  
C 5.38222317 -1.35924204 0.78322784

H 3.42595648 -0.74649923 1.37096331  
C 6.49749756 0.02193016 -0.85383807  
H 5.39016718 1.70909699 -1.55426396  
C 6.50063929 -1.08891501 -0.01098307  
H 5.38840766 -2.21332935 1.45486384  
H 7.37160048 0.22739593 -1.45967141  
O -7.32678181 -2.28313842 -0.28787031  
O 0.17734688 -3.41981908 2.41896128  
O 0.84902680 -3.04635542 -2.35385819  
O 0.19820969 5.84021761 0.15713918  
O 7.62337878 -1.87072095 0.00496686  
O -2.87070614 2.19356405 0.02426278  
H -8.12142188 -1.74131912 -0.23207703  
H 0.58664325 -4.28098732 2.28507732  
H 1.29432098 -3.89201029 -2.23713016  
H 7.51633151 -2.58269719 0.64428124

### Cartesian coordinates RAF 11b

C 1.67078509 2.44923234 -0.29838612  
C 0.64261327 1.46074405 -0.28527416  
C -0.73525686 1.89093023 -0.40693625  
C -0.96397785 3.22964125 -0.50387305  
C 0.09012524 4.29541957 -0.44655998  
C 1.48899312 3.78580019 -0.39349303  
C 2.66839110 0.47493499 -0.10668425  
C 1.29680706 0.21250912 -0.15719210  
H -1.97631933 3.59556732 -0.63996421  
H 2.30019592 4.50022440 -0.43427090  
C 3.85740739 -0.34043190 0.02577622  
C 5.12882664 0.25617788 -0.09481586  
C 3.80639735 -1.72651010 0.28640184  
C 6.28926473 -0.49362606 0.03045521  
H 5.20045343 1.31729098 -0.29152586  
C 4.96338943 -2.47622038 0.41335411  
H 2.85270618 -2.22119028 0.39873823  
C 6.21328069 -1.86517835 0.28388084  
H 7.25713256 -0.01106880 -0.06972810  
H 4.91710653 -3.53900515 0.61714027  
C 0.65331588 -1.12617915 -0.08779580  
C 0.12604579 -1.57586286 1.12464612

C 0.56634719 -1.92020590 -1.23523729  
 C -0.48683778 -2.82647221 1.18570524  
 H 0.17765592 -0.96703226 2.01762214  
 C -0.04846523 -3.16871707 -1.15889130  
 H 0.96944796 -1.58391217 -2.18175811  
 C -0.57540723 -3.63191227 0.04831812  
 H -1.05060417 -4.60829721 0.10180418  
 C -1.83668533 0.91677895 -0.45086378  
 H -1.62691735 -0.02031723 -0.95507709  
 C -3.04539126 1.11639095 0.10276199  
 H -3.19649835 2.02004101 0.68899619  
 C -4.19918816 0.21497720 0.04273583  
 C -4.29781251 -0.85401800 -0.86289230  
 C -5.27762547 0.41700808 0.92173310  
 C -5.40753160 -1.68953701 -0.87577829  
 H -3.50537329 -1.02937305 -1.58091439  
 C -6.39199867 -0.41116120 0.92018791  
 H -5.23537860 1.24086032 1.62654799  
 C -6.45932959 -1.47271087 0.01871224  
 H -5.46480763 -2.50414929 -1.59261397  
 H -7.21561067 -0.24645107 1.60426327  
 O 7.31846685 -2.65561146 0.41708481  
 O -0.10972014 -3.90732839 -2.30886701  
 O -0.98170582 -3.22013405 2.39628127  
 O -0.00695921 5.21545825 -1.51015386  
 O -7.57841935 -2.26118444 0.04733914  
 O 2.89236007 1.83151209 -0.19901615  
 H 8.11573640 -2.12630192 0.30773721  
 H -1.43601295 -4.06476709 2.31188809  
 H -0.89328506 5.60037861 -1.49477703  
 H -0.53480928 -4.75365056 -2.13583822  
 H -7.51920759 -2.93487100 -0.63796710  
 O -0.18356312 5.19446738 0.70727185  
 O -0.25014103 4.42034245 1.92743923  
 H 0.64295089 4.54503936 2.28067510

**Cartesian coordinates RAF 2b**

C 1.73943790 2.78984521 0.02990486  
 C 0.84407317 1.70622197 0.02199896  
 C -0.55290820 1.98009131 0.01687176

C -0.92963213 3.33996306 0.03306511  
 C 0.00222889 4.37769552 0.04924206  
 C 1.37617095 4.12262045 0.04639509  
 C 2.98132429 0.96056730 0.02296682  
 C 1.67885134 0.52177088 0.02126287  
 H -1.98238635 3.59723952 -0.00627287  
 H 2.09892123 4.92700850 0.04886899  
 C 4.28729935 0.31023122 0.02385002  
 C 5.44410569 1.06747698 -0.22828019  
 C 4.44705849 -1.06375634 0.28360990  
 C 6.70291570 0.47977485 -0.23005610  
 H 5.35368729 2.12721528 -0.42592418  
 C 5.70130435 -1.65438906 0.28397292  
 H 3.58431754 -1.67806604 0.49827806  
 C 6.83735371 -0.88564110 0.02495600  
 H 7.58145260 1.08610984 -0.43063810  
 H 5.81766355 -2.71146824 0.48974508  
 C 1.22745785 -0.89451487 0.01210916  
 C 0.83873324 -1.50808637 1.20731207  
 C 1.18843526 -1.60746003 -1.18955923  
 C 0.41820190 -2.83649113 1.19418901  
 H 0.86313413 -0.96951305 2.14572326  
 C 0.76770919 -2.93674746 -1.18813416  
 H 1.48751090 -1.14680595 -2.12197696  
 C 0.37941585 -3.56025003 -0.00032809  
 H 0.05490902 -4.59793433 -0.00378520  
 C -1.53067006 0.91533694 -0.03117224  
 H -1.14096595 -0.06719916 -0.26131725  
 C -2.87918726 1.04889016 0.19559291  
 H -3.25738919 2.02329704 0.48854279  
 C -3.86659338 0.03572793 0.10093897  
 C -3.61890721 -1.28758985 -0.31391112  
 C -5.29034953 0.44380614 0.41315620  
 C -4.61208612 -2.23763711 -0.35535099  
 H -2.61561413 -1.57278516 -0.60758227  
 C -6.28072328 -0.67145925 0.46323594  
 H -5.32465133 1.03075314 1.33870625  
 C -5.95197244 -1.91857022 0.06340178  
 H -4.38898922 -3.24376234 -0.69784826

H -7.28450954 -0.45612115 0.80661694  
 O 8.04729844 -1.52185291 0.03834418  
 O 0.75402307 -3.58912352 -2.38976816  
 O 0.05655317 -3.38947130 2.39074238  
 O -0.37642812 5.69399959 0.05269600  
 O -6.90993566 -2.90206413 0.06791514  
 O 3.02369128 2.34328629 0.02486498  
 H 8.75072688 -0.89058203 -0.14652124  
 H -0.21931804 -4.30326039 2.26522630  
 H -1.33733886 5.75591438 0.04295014  
 H 0.46907700 -4.50088322 -2.26963540  
 H -6.50759955 -3.74920917 -0.14688479  
 O -5.60992867 1.40855236 -0.65788427  
 O -6.81541349 2.12591139 -0.26907023  
 H -7.45578464 1.76158926 -0.89644901

**Cartesian coordinates RAF 2b**

C -2.28605524 2.73720107 -0.07376995  
 C -1.20501333 1.84008529 -0.01775178  
 C 0.11799912 2.37035900 0.00032015  
 C 0.23185584 3.77873726 -0.03285291  
 C -0.87634927 4.62209656 -0.08413389  
 C -2.17856294 4.11369534 -0.10733196  
 C -3.16701206 0.70929013 -0.03601792  
 C -1.80527390 0.52184709 0.00841498  
 H 1.21717911 4.23114729 -0.03550091  
 H -3.03841617 4.76795157 -0.15145582  
 C -4.33118719 -0.16978705 -0.04105886  
 C -5.61543052 0.37557720 -0.21379078  
 C -4.23017731 -1.56385424 0.12786616  
 C -6.74573037 -0.43169804 -0.22336519  
 H -5.72745947 1.44364792 -0.34237821  
 C -5.35550448 -2.37319645 0.11950886  
 H -3.26356204 -2.02381193 0.27302900  
 C -6.62124672 -1.81174203 -0.05754485  
 H -7.72629052 0.01483284 -0.36056391  
 H -5.26957827 -3.44478514 0.25205083  
 C -1.09753796 -0.78451215 0.06952119  
 C -0.80316618 -1.47457304 -1.11007417  
 C -0.72208617 -1.31426832 1.30784622

C -0.14150305 -2.70008405 -1.04306921  
H -1.08698034 -1.07716410 -2.07581418  
C -0.05932712 -2.53962322 1.36046391  
H -0.94155608 -0.79081889 2.22929728  
C 0.23462185 -3.24109635 0.18848976  
H 0.74616691 -4.19933739 0.23533412  
C 1.27059903 1.50356613 0.03825105  
H 1.06017011 0.44586623 -0.03281111  
C 2.58751429 1.89507792 0.16108526  
H 2.80382396 2.95488448 0.26408802  
C 3.72317523 1.05589912 0.17841423  
C 3.66338720 -0.38137328 0.05556414  
C 5.02870948 1.64001608 0.34200726  
C 4.77362541 -1.14611114 0.04808422  
H 2.69588132 -0.86316006 -0.02272975  
C 6.16487473 0.91107018 0.35128691  
H 5.08924630 2.71528520 0.48085913  
C 6.15775254 -0.57188979 0.15541724  
H 4.70224734 -2.22602114 -0.02329809  
H 7.13896040 1.36010407 0.49828811  
O -7.69396150 -2.65848543 -0.05761311  
O 0.27684490 -3.01448836 2.59632721  
O 0.11552627 -3.33703248 -2.22508397  
O -0.75332932 5.98603240 -0.12179120  
O 6.89982256 -1.17325422 1.19323596  
O -3.46380853 2.05935941 -0.08777516  
H -8.50644384 -2.15727519 -0.18480192  
H 0.55552922 -4.17746332 -2.06051990  
H 0.17774376 6.23021225 -0.10171475  
H 0.75089193 -3.84870243 2.51633201  
H 7.05367978 -2.09446926 0.94371989  
O 6.88303864 -0.73789322 -1.10261700  
O 7.08009843 -2.17161008 -1.32225202  
H 6.53721231 -2.30620419 -2.11152729

**Cartesian coordinates RAF 7a**

C -1.58315016 2.63559110 0.36408294  
C -0.53207979 1.67708335 0.26944277  
C 0.78540487 2.14965504 -0.03031709  
C 0.96146532 3.54134940 -0.12506787

C -0.09526990 4.43612727 0.03661483  
C -1.40857935 3.99092940 0.27216115  
C -2.60739813 0.62696497 0.68434789  
C -1.11175695 0.40603029 0.47097781  
H 1.93612408 3.93274054 -0.39649399  
H -2.22848234 4.68960847 0.36521803  
C -3.59022527 -0.07924112 -0.22763618  
C -4.83893858 -0.49685193 0.23286127  
C -3.29214343 -0.22593699 -1.58690520  
C -5.76225657 -1.06523909 -0.63992823  
H -5.09000938 -0.38304707 1.27849435  
C -4.20714328 -0.78776606 -2.46751594  
H -2.33124592 0.10533114 -1.96547596  
C -5.44816448 -1.21327114 -1.99121197  
H -6.72810348 -1.39348615 -0.26677677  
H -3.97706654 -0.90301399 -3.51961715  
C -0.44877088 -0.87085694 0.76322811  
C -0.86503282 -2.07503417 0.17185719  
C 0.60274506 -0.89260295 1.70027190  
C -0.22622909 -3.26598832 0.50253000  
H -1.67846292 -2.10206031 -0.53832514  
C 1.22339906 -2.09435337 2.02499305  
H 0.93532026 0.01559274 2.18448443  
C 0.81976594 -3.29148302 1.42841185  
H 1.30858813 -4.22810135 1.68413517  
C 1.87685517 1.22595287 -0.31261993  
H 1.57437111 0.22630900 -0.60125119  
C 3.19512513 1.50687931 -0.23978926  
H 3.50034504 2.47934623 0.13934877  
C 4.30067642 0.61528815 -0.58385396  
C 4.13209219 -0.59973616 -1.27091812  
C 5.61311855 0.97480799 -0.22558614  
C 5.21405964 -1.41623919 -1.57068010  
H 3.14432306 -0.90934295 -1.59074914  
C 6.70298873 0.16710200 -0.51858312  
H 5.77810226 1.90927892 0.30089018  
C 6.50597763 -1.03715883 -1.19383022  
H 5.05727818 -2.34649099 -2.10952118  
H 7.70807360 0.45475429 -0.23493988

O -6.31382225 -1.76658734 -2.89443339  
O 2.22665615 -2.04760691 2.95378909  
O -0.66774919 -4.40230121 -0.11941308  
O 0.07547920 5.78667228 -0.06431885  
O 7.60856658 -1.79987629 -1.46657717  
O -2.79211432 2.04572410 0.54605324  
H -7.12965958 -2.01969916 -2.44980226  
H -0.17190005 -5.16518324 0.19488698  
H 1.00502190 5.98677325 -0.21858090  
H 2.59449202 -2.92696245 3.08867848  
H 7.34747635 -2.58933096 -1.95219837  
O -2.95669744 0.47397295 2.09530219  
O -2.93160809 -0.92429908 2.46672800  
H -2.04350103 -1.01061318 2.84651004

**Cartesian coordinates RAF 7a**

C -1.67303039 2.73267343 -0.15142513  
C -0.72385098 1.70811695 -0.02957095  
C 0.67115921 2.06132319 -0.00960880  
C 0.96484623 3.45584335 -0.10253127  
C -0.02443000 4.42206651 -0.21117876  
C -1.38636131 4.08297449 -0.24492228  
C -2.81153301 0.83989531 -0.06193226  
C -1.48215086 0.48359127 0.02296206  
H 1.99867813 3.77362223 -0.03773193  
H -2.15289837 4.84059861 -0.33198781  
C -4.07462407 0.11287986 -0.06632178  
C -5.27529920 0.80084891 -0.31619822  
C -4.15257717 -1.27155102 0.17909898  
C -6.49611059 0.13846081 -0.32617798  
H -5.24880436 1.86551438 -0.50541878  
C -5.36895564 -1.93626432 0.17031676  
H -3.25471843 -1.83613922 0.38501085  
C -6.54890237 -1.23485734 -0.08358408  
H -7.40921651 0.69254697 -0.52360925  
H -5.42128068 -3.00096524 0.36267322  
C -0.93923194 -0.89674324 0.12109375  
C -0.72636615 -1.63928422 -1.04321791  
C -0.63027497 -1.44202705 1.37130992  
C -0.20902978 -2.93027245 -0.95137814



H	-0.95682602	-1.22868819	-2.01752319	C	0.70170226	4.11326354	-0.49492202	O	0.00421596	-4.03329744	-0.71438505
C	-0.11432187	-2.73425726	1.44787235	C	2.37736848	0.99209621	-0.30732286	O	0.44963238	-2.51812910	3.85361213
H	-0.78814707	-0.87787383	2.28138631	C	1.16973943	0.59430309	0.20592615	O	-1.02469089	5.69736727	-0.24344482
C	0.09748503	-3.48782947	0.29147083	H	-2.46006089	3.66236801	0.66830694	O	-5.68511047	-2.71016011	-3.01855721
H	0.49847015	-4.49625239	0.35748728	H	1.35203835	4.87864434	-0.89642732	O	2.34527547	2.33524809	-0.64379387
C	1.68842891	1.09967107	0.08835514	C	3.65312222	0.32955783	-0.56428710	H	7.86158368	-1.02831416	-1.91375841
H	1.42200510	0.06043575	0.21146981	C	4.58656972	0.92333916	-1.42964801	H	0.16553405	-3.41673504	4.04991308
C	3.15044405	1.41844586	-0.00112503	C	4.00148331	-0.89222512	0.03957611	H	-1.93012586	5.77937070	0.07289999
H	3.34277405	2.12248338	-0.81950400	C	5.80970261	0.31834986	-1.69259724	H	-0.13759878	-4.88225915	-0.28286694
C	4.02240751	0.19460017	-0.18761186	H	4.34915752	1.86767607	-1.90157410	H	-5.10378809	-3.45808548	-3.19289306
C	4.17991553	-0.73209397	0.84714292	C	5.22088867	-1.49971214	-0.21922120	O	-2.09487726	1.32406233	2.49251639
C	4.68854641	-0.03809177	-1.39380525	H	3.31872136	-1.36835235	0.72929409	O	-2.73770696	0.19372491	3.14120409
C	4.97917056	-1.86015593	0.68232009	C	6.13119683	-0.89842390	-1.08991622	H	-3.66521339	0.47264313	3.15117326
H	3.67798614	-0.56647684	1.79426701	H	6.51392957	0.79527932	-2.36817032	<b>Cartesian coordinates RAF 10b</b>			
C	5.48210061	-1.16566688	-1.57654391	H	5.48620650	-2.43751794	0.25348596	C	1.44977791	2.57591525	-0.26972588
H	4.58786515	0.67454012	-2.20593516	C	0.82913238	-0.77025294	0.68451300	C	0.55990181	1.51687918	-0.09591391
C	5.63008821	-2.07967294	-0.53375781	C	0.77545105	-1.02985407	2.05707707	C	-0.84000221	1.76536123	-0.09252876
H	5.09677649	-2.56779397	1.49831299	C	0.56977732	-1.79214236	-0.23599030	C	-1.28130693	3.21365745	-0.09646319
H	5.99816855	-1.34480132	-2.51195836	C	0.47104237	-2.31454403	2.50410802	C	-0.21121687	4.25029822	-0.34272905
O	-7.71865079	-1.94271393	-0.07930727	H	0.95907026	-0.24776925	2.78202503	C	1.10496126	3.94056548	-0.41817915
O	0.16941292	-3.22290747	2.69433242	C	0.26214806	-3.07019009	0.22626190	C	2.69572733	0.75643824	-0.14138081
O	-0.02241119	-3.61332439	-2.12055717	H	0.61287404	-1.60721608	-1.30154319	C	1.39564520	0.33054422	-0.02141104
O	0.26660796	5.75871320	-0.28479896	C	0.21282133	-3.34257244	1.59402634	H	-2.09360829	3.35893936	-0.82154609
O	6.42713074	-3.17100523	-0.75768181	H	-0.02765692	-4.34206761	1.94786600	H	1.85621726	4.70202932	-0.58206322
O	-2.92993801	2.21175823	-0.16998179	C	-1.98736326	1.02578099	1.06866710	C	4.00357250	0.11132778	-0.12483820
H	-8.45804265	-1.35306019	-0.26118019	H	-1.53228723	0.04196587	0.98526295	C	5.13888525	0.81745926	-0.55756020
H	0.36793588	-4.47518955	-1.94261127	C	-3.33135123	1.05440895	0.41421296	C	4.18642758	-1.20877895	0.32733793
H	1.21870103	5.88503840	-0.21203127	H	-3.93327818	1.93916685	0.60203808	C	6.39823237	0.23019210	-0.55032899
H	0.49111300	-4.12789529	2.62837418	C	-3.88004507	0.06997681	-0.43467201	H	5.03178824	1.83659696	-0.90469783
H	6.48227842	-3.70355652	0.04257019	C	-3.20767510	-1.13182018	-0.79806015	C	5.44101635	-1.79936828	0.33509091
O	3.47566422	2.11910035	1.23556326	C	-5.18041719	0.26233803	-0.99286617	H	3.34112725	-1.77819325	0.68708797
O	4.78607113	2.73511029	1.08032382	C	-3.78984098	-2.05642142	-1.64722029	C	6.55473231	-1.08327504	-0.10630324
H	5.37084533	2.05033429	1.43847998	H	-2.21689283	-1.33836494	-0.41548299	H	7.25979644	0.79644086	-0.89229286

**Cartesian coordinates RAF 8b**

C	1.10807599	2.80214911	-0.32932023	C	-5.76099713	-0.66091593	-1.83672713	H	5.57496857	-2.81465198	0.68816697
C	0.31199814	1.76847914	0.19848222	H	-5.72419338	1.16745180	-0.74339402	C	0.94373629	-1.07218984	0.16263786
C	-1.02055008	2.07484208	0.54376719	C	-5.06698540	-1.83103795	-2.17399508	C	0.52189418	-1.50570401	1.42382706
C	-1.44509681	3.39666546	0.39302523	H	-3.24636431	-2.95997252	-1.90940434	C	0.93712211	-1.95427539	-0.92216703
C	-0.60323296	4.40021149	-0.10551212	H	-6.74845722	-0.49886016	-2.25221224	C	0.10427491	-2.82381310	1.59498891
				O	7.31761487	-1.54293428	-1.30824205	H	0.51731680	-0.83355418	2.27201141

C 0.51822698 -3.27056200 -0.73641206  
H 1.25794587 -1.63329817 -1.90454808  
C 0.10001397 -3.71576411 0.51947425  
H -0.22247617 -4.74468047 0.65929823  
C -1.82011097 0.74714483 -0.13640708  
H -1.43761213 -0.26461826 -0.18789020  
C -3.18292707 0.92239828 -0.14040713  
H -3.57955812 1.92694392 -0.03795894  
C -4.18577034 -0.11849602 -0.24914882  
C -3.88742021 -1.49090134 -0.37897505  
C -5.55177050 0.23869228 -0.22792775  
C -4.89188436 -2.44218793 -0.48102318  
H -2.85678825 -1.82358925 -0.40134178  
C -6.56227732 -0.70420897 -0.33037224  
H -5.81684438 1.28604095 -0.12789420  
C -6.23557228 -2.05509636 -0.45811509  
H -4.63381837 -3.49286618 -0.58210291  
H -7.60573178 -0.41348481 -0.31359890  
O 7.76730864 -1.71658220 -0.07594117  
O 0.53607296 -4.09305320 -1.82952503  
O -0.28915197 -3.19797528 2.84991000  
O -0.63071525 5.53191524 -0.49868500  
O -7.26513742 -2.95131518 -0.55807985  
O 2.72776319 2.13343206 -0.30032396  
H 8.45390660 -1.12100432 -0.39401321  
H -0.55631505 -4.12286757 2.85201719  
H -1.52327587 5.60709440 -0.12474084  
H 0.24474977 -4.97706655 -1.58364018  
H -6.91327636 -3.84262112 -0.65207390  
O -1.88846426 3.42917547 1.22275823  
O -2.71479306 4.65903261 1.11576123  
H -2.66490805 4.95785212 2.03460820

**Cartesian coordinates RAF 11a**

C 1.57483308 3.04219026 -0.24209012  
C 0.57828701 2.05134238 -0.20637278  
C -0.77986121 2.45502418 -0.26369008  
C -1.02388230 3.83250114 -0.38170984  
C 0.00460384 4.78108628 -0.41620214  
C 1.34321590 4.40173710 -0.34420281

C 2.63278329 1.10824533 -0.04327823  
C 1.29677425 0.79675308 -0.07048906  
H -2.04778207 4.17691932 -0.48400403  
H 2.14083525 5.13126033 -0.37490197  
C 3.86852541 0.34213108 0.09115025  
C 5.07117913 1.00692112 0.38510292  
C 3.91397644 -1.05552499 -0.06737908  
C 6.26373827 0.30812986 0.52555080  
H 5.06905925 2.08191136 0.50647025  
C 5.10171531 -1.75734526 0.07298307  
H 3.01775497 -1.60478187 -0.31766087  
C 6.28393538 -1.07891303 0.37285088  
H 7.17982453 0.84453302 0.75547408  
H 5.12833663 -2.83254029 -0.05507624  
C 0.70871121 -0.56159888 0.07379483  
C 0.50787310 -1.08893089 1.37342399  
C 0.34415677 -1.28907102 -1.02669118  
C -0.06450724 -2.37770609 1.55122013  
H 0.78992881 -0.51853391 2.24861119  
C -0.26286721 -2.65353233 -0.91719223  
H 0.47109211 -0.90635998 -2.03137705  
C -0.43754809 -3.14107814 0.48939900  
H -0.84593905 -4.13789621 0.61802981  
C -1.87793840 1.48707591 -0.21598105  
H -1.62739837 0.47762586 -0.51732103  
C -3.13785810 1.75256996 0.18104900  
H -3.36586417 2.74954942 0.55116298  
C -4.27132931 0.82773323 0.20395497  
C -4.22701124 -0.47178427 -0.33168883  
C -5.48335635 1.24698290 0.78172392  
C -5.33600959 -1.30566813 -0.28188690  
H -3.32348025 -0.84441607 -0.79982125  
C -6.59839155 0.42158228 0.83604502  
H -5.54964162 2.24634208 1.19977712  
C -6.52712831 -0.86393795 0.30195224  
H -5.27997131 -2.30439441 -0.70635796  
H -7.52565985 0.75734313 1.28420894  
O 7.42515374 -1.82153234 0.49937504  
O -1.48739924 -2.64582433 -1.63329500

O -0.19732808 -2.77253635 2.85528115  
O -0.25416595 6.12201032 -0.53840398  
O -7.64931481 -1.64490091 0.37172691  
O 2.80866223 2.47710516 -0.14777804  
H 8.16996861 -1.24412429 0.69748101  
H -0.58436514 -3.65383238 2.89300302  
H -1.20537423 6.26500036 -0.57641902  
H -1.86972927 -3.52985303 -1.55749935  
H -7.47730152 -2.49835798 -0.03941894  
O 0.69580405 -3.49269843 -1.62255799  
O 0.13338495 -4.84460343 -1.68870991  
H 0.13760090 -4.97303951 -2.64754945

**Cartesian coordinates RAF 12b**

C 1.57938824 2.35668823 -0.27390902  
C 0.54045507 1.46585220 -0.17997477  
C -0.82667488 1.94797607 -0.23661526  
C -0.96767627 3.37075324 -0.40998325  
C 0.07438486 4.23699629 -0.48240486  
C 1.51429309 3.83019128 -0.34603906  
C 2.52332033 0.37243495 -0.13668013  
C 1.16653791 0.15659995 -0.08891712  
H -1.96773925 3.77931829 -0.51330405  
H 2.10517240 4.23761013 -1.17827135  
C 3.70853449 -0.48262500 -0.10291386  
C 4.94249540 0.01373215 -0.55332890  
C 3.66889012 -1.80181202 0.38161617  
C 6.08632472 -0.77528118 -0.53167708  
H 5.00523518 1.02801200 -0.92557281  
C 4.80724828 -2.59439730 0.40351988  
H 2.74158530 -2.21216622 0.75661922  
C 6.02276736 -2.08537641 -0.05537893  
H 7.02873278 -0.36961285 -0.88817109  
H 4.77120548 -3.60877240 0.78182023  
C 0.50311897 -1.17019293 0.00632896  
C 0.02097606 -1.62583518 1.23849014  
C 0.37600584 -1.96616336 -1.13492803  
C -0.57791289 -2.88108913 1.32230335  
H 0.11197020 -1.02160631 2.13190908  
C -0.22636615 -3.21966044 -1.03737897

H	0.74362527	-1.62835618	-2.09491801	C	-1.28841600	0.52608000	0.03167800	O	0.22471100	5.88216900	0.14633300
C	-0.70681094	-3.68655141	0.18788279	H	2.02909800	3.94798700	0.25548200	O	7.63046400	-1.94998600	0.08369500
H	-1.17047710	-4.66748833	0.25933178	H	-2.16339400	4.86820500	0.05085100	O	-2.81550400	2.19815400	0.00924900
C	-1.93874192	1.07605706	-0.16489904	C	-3.85664500	0.04190700	-0.07255300	H	-8.16769100	-1.63244800	-0.06555400
H	-1.70088310	0.02370079	-0.08211402	C	-5.09353400	0.66188800	0.17167800	H	1.31851400	-3.94388900	-2.22959700
C	-3.26972007	1.42715029	-0.18704087	C	-3.86171100	-1.32995900	-0.38569100	H	1.17496200	6.03310100	0.17543600
H	-3.53510617	2.47839000	-0.24557105	C	-6.28181800	-0.05668200	0.11810100	H	0.31146900	-4.43405200	2.21929000
C	-4.40339131	0.52796914	-0.13219694	H	-5.12219100	1.71723100	0.40798500	H	7.46591300	-2.72125800	0.63601700
C	-4.29333514	-0.87753410	-0.07375620	C	-5.04481600	-2.05114200	-0.44032500				
C	-5.70972621	1.06587093	-0.13849098	H	-2.93257400	-1.83903800	-0.59930000				
C	-5.41779235	-1.68817121	-0.02301974	C	-6.26253900	-1.41825300	-0.18587800	C	1.58547600	2.78824700	0.00006300
H	-3.31718251	-1.34671324	-0.06915976	H	-7.22518400	0.44489900	0.31394600	C	0.57507100	1.79122800	0.00004200
C	-6.83848033	0.26402399	-0.08795296	H	-5.04171000	-3.10602300	-0.68650700	C	-0.80449600	2.21345300	-0.00000800
H	-5.83230535	2.14316839	-0.18274713	C	-0.68342500	-0.83101300	0.02613200	C	-1.03212600	3.60462600	-0.00009500
C	-6.69730748	-1.12345124	-0.02947888	C	-0.14408000	-1.34381800	-1.15768200	C	0.00457800	4.53271400	-0.00008200
H	-5.30430658	-2.76799231	0.02021087	C	-0.64700900	-1.58829500	1.20091000	C	1.36402400	4.13377200	-0.00000400
H	-7.83321978	0.69295390	-0.09274784	C	0.42265800	-2.61651900	-1.16233300	C	2.63345600	0.84828200	0.00011000
O	7.11204168	-2.91161630	-0.01039992	H	-0.16017500	-0.76785000	-2.07371400	C	1.25676700	0.54737600	0.00002700
O	-0.32053113	-3.95837653	-2.18386635	C	-0.07820800	-2.86072400	1.18157600	H	-2.04835200	3.97948400	-0.00019000
O	-1.02195716	-3.28207848	2.55215625	H	-1.06093400	-1.20545000	2.12462900	H	2.15789600	4.86808600	-0.00000900
O	-0.05453701	5.57645768	-0.68567983	C	0.45865400	-3.38471500	0.00399000	C	3.83290100	0.05996400	0.00011500
O	-7.83893754	-1.87651597	0.01810580	H	0.89804100	-4.37919100	-0.00569200	C	5.09129100	0.71058300	0.00006100
O	2.77722539	1.72078122	-0.25188202	C	1.87106000	1.24352800	0.20238300	C	3.81631300	-1.35694300	0.00017600
H	7.88757581	-2.44745430	-0.34272588	H	1.60821900	0.26043100	0.57434100	C	6.26654200	-0.01142600	0.00007400
H	-1.40005589	-4.16571823	2.49689322	C	3.14314300	1.47780700	-0.17373300	H	5.13302600	1.79106600	-0.00000100
H	-0.98714999	5.82042744	-0.68876017	H	3.38275900	2.43603100	-0.62890500	C	4.98874900	-2.08028500	0.00019000
H	-0.73819380	-4.80593856	-1.99939093	C	4.27420400	0.55446600	-0.07320500	H	2.87685900	-1.88827200	0.00023200
H	-7.61178080	-2.81142347	0.05533395	C	4.23462000	-0.64309800	0.66120500	C	6.22515600	-1.41530500	0.00015000
O	2.18349434	4.50124359	0.76120507	C	5.47802200	0.86638100	-0.73032400	H	7.22120600	0.50428400	0.00000600
O	1.52353623	4.14632124	2.00357196	C	5.33441700	-1.48862700	0.72309500	H	4.97940000	-3.16282500	0.00025000
H	2.15581731	3.51498420	2.37660011	H	3.33780400	-0.91607300	1.20446300	C	0.66490100	-0.81655600	-0.00008500

### Cartesian coordinates Vam3 radical cation

### Cartesian coordinates Vam3

C	-1.58624300	2.77765700	0.05608100	C	6.58436700	0.02950100	-0.67692700	C	0.39245500	-1.45002400	1.21491000
C	-0.58276300	1.79388800	0.07957000	H	5.54313100	1.78684800	-1.30141500	C	0.39252200	-1.44985600	-1.21517400
C	0.77106700	2.20823400	0.13819700	C	6.51507900	-1.15676400	0.05230500	C	-0.14920000	-2.73792500	1.20687500
C	1.00847400	3.59168800	0.16042100	H	5.28147600	-2.40438000	1.30554200	H	0.60199100	-0.97224500	2.16320400
C	-0.02562700	4.53391500	0.11756600	H	7.50496400	0.28134700	-1.18929100	C	-0.14913900	-2.73776300	-1.20734900
C	-1.36191300	4.14240200	0.06815000	O	-7.39746000	-2.17923200	-0.25294800	H	0.60211300	-0.97195300	-2.16339400
C	-2.62657400	0.82555900	-0.00982700	O	-0.07037300	-3.56116700	2.35749400	C	-0.42279400	-3.38667100	-0.00029100
				O	0.92751700	-3.07221200	-2.34824200	H	-0.83704800	-4.39132900	-0.00037000

C	-1.86358200	1.24342900	0.00005300
H	-1.55105900	0.20920800	0.00015100
C	-3.20322800	1.51588100	0.00002400
H	-3.52646500	2.55283600	-0.00000200
C	-4.27909000	0.56084800	0.00004500
C	-4.08418900	-0.84297100	0.00006600
C	-5.60992600	1.03644300	0.00007900
C	-5.15215700	-1.71173500	0.00012400
H	-3.08154800	-1.25187000	0.00003900
C	-6.68962700	0.17284800	0.00013300
H	-5.78945800	2.10599900	0.00005500
C	-6.46625600	-1.21086600	0.00016700
H	-5.00818500	-2.78490100	0.00014300
H	-7.70261300	0.56161300	0.00015000
O	7.33132500	-2.18100300	0.00015400
O	-0.38807000	-3.30931900	-2.41730000
O	-0.38819000	-3.30966300	2.41672800
O	-0.20119200	5.86552400	-0.00017700
O	-7.46298800	-2.11851700	0.00022800
O	2.81564900	2.20439400	0.00010900
H	8.13212700	-1.64220400	0.00016200
H	-0.72441600	-4.20700800	2.31499500
H	-1.14270400	6.07636500	-0.00025900
H	-0.72425100	-4.20669800	-2.31572100
H	-8.32713700	-1.68915800	0.00025700

**Cartesian coordinates RAF TS 4b**

C	-2.32824600	2.72425300	-0.06509600
C	-1.23803500	1.83949900	0.01666900
C	0.07395200	2.38452900	0.07658400
C	0.17790000	3.79001100	0.03710700
C	-0.93740500	4.62303100	-0.05369700
C	-2.23263500	4.10104400	-0.10504700
C	-3.18349700	0.68479300	-0.05943600
C	-1.82185100	0.51316600	0.01373700
H	1.15695000	4.25105000	0.10887200
H	-3.09782900	4.74690200	-0.16706500
C	-4.33476800	-0.21008300	-0.09771900
C	-5.63402900	0.32117100	-0.02320600
C	-4.20369000	-1.60685600	-0.21405400

C	-6.75168000	-0.50294100	-0.05649600
H	-5.76755600	1.39110800	0.06252400
C	-5.31620300	-2.43292800	-0.24869800
H	-3.22302900	-2.05483400	-0.28424600
C	-6.59798200	-1.88548900	-0.16838900
H	-7.74501100	-0.06797600	0.00479500
H	-5.20788100	-3.50671800	-0.34068300
C	-1.09116200	-0.78056500	0.06840800
C	-0.59119800	-1.34179200	-1.11015600
C	-0.88553000	-1.41867000	1.29536400
C	0.11258100	-2.54418500	-1.05691200
H	-0.73744500	-0.85642800	-2.06630800
C	-0.18262800	-2.62247000	1.33389600
H	-1.26494200	-0.99571600	2.21646000
C	0.31985400	-3.19342900	0.16262200
H	0.86409600	-4.13378600	0.19892200
C	1.23752300	1.52736900	0.19905600
H	1.02484900	0.48601600	0.39816400
C	2.54355800	1.90502900	0.07799400
H	2.76765300	2.93414400	-0.18945000
C	3.69333700	1.06565400	0.24371800
C	3.62223400	-0.29063000	0.68550100
C	4.98836600	1.60612900	-0.01094600
C	4.74443700	-1.05328200	0.83040700
H	2.66085700	-0.71995200	0.93927200
C	6.12156300	0.85660300	0.12154800
H	5.06636500	2.64615100	-0.31044900
C	6.03643900	-0.54171200	0.46366900
H	4.69828500	-2.07198100	1.19475600
H	7.10181800	1.27907300	-0.06609700
O	-7.65694400	-2.74840800	-0.20631500
O	-0.01401400	-3.20793500	2.55784600
O	0.57278700	-3.04938400	-2.23856200
O	-0.82650100	5.98811200	-0.08336700
O	7.10810000	-1.16777000	1.02578600
O	-3.49709300	2.03221200	-0.10514700
H	-8.48261000	-2.25634100	-0.14562000
H	1.11160800	-3.83173000	-2.08136100
H	0.10163600	6.24095900	-0.04443400

**Cartesian coordinates RAF TS 7b**

C	-1.70904100	2.72340000	-0.18775500
C	-0.75072500	1.69976600	-0.10640200
C	0.62928200	2.06041600	-0.10892400
C	0.92433000	3.44037300	-0.18654900
C	-0.06941100	4.41407100	-0.25824200
C	-1.42622600	4.07368200	-0.26660400
C	-2.83653500	0.82309700	-0.10104200
C	-1.50755900	0.46877400	-0.05593600
H	1.95836700	3.75634300	-0.11435700
H	-2.19648900	4.83115600	-0.31706800
C	-4.09955900	0.09389300	-0.08462600
C	-5.31323300	0.80148300	-0.03127700
C	-4.16306500	-1.31188900	-0.12649000
C	-6.53357000	0.13804100	-0.01602200
H	-5.29795300	1.88255200	-0.00048800
C	-5.37866500	-1.97797900	-0.11211200
H	-3.25418200	-1.89371000	-0.17559400
C	-6.57223800	-1.25630200	-0.05567000
H	-7.45708400	0.70812000	0.02739700
H	-5.41951900	-3.05985600	-0.14631800
C	-0.95863300	-0.91050000	0.02407200
C	-0.59953200	-1.58146000	-1.14855100
C	-0.79451300	-1.52817600	1.26755200
C	-0.08531300	-2.87444500	-1.07195500
H	-0.71730900	-1.11435900	-2.11761800
C	-0.28062700	-2.82273300	1.32911100
H	-1.06705500	-1.02085200	2.18384400
C	0.07580400	-3.50488800	0.16398100
H	0.47311400	-4.51549500	0.21772500
C	1.67037400	1.07703700	-0.02094700
H	1.37819300	0.08652400	0.30043700
C	3.02033500	1.30759300	-0.30134500
H	3.25923600	2.16052000	-0.92699800

C	4.01406700	0.22707600	-0.34378500
C	3.91919500	-0.91683000	0.46311000
C	5.13706000	0.34416800	-1.18109800
C	4.89359600	-1.90971600	0.41967300
H	3.08420100	-1.03175300	1.14330000
C	6.11084200	-0.64180100	-1.23780400
H	5.24307600	1.22704000	-1.80245400
C	5.98987500	-1.77764600	-0.43443200
H	4.80408400	-2.78444000	1.05768400
H	6.96893900	-0.54797700	-1.89214100
O	-7.74035100	-1.96649400	-0.04323500
O	-0.14487100	-3.38356300	2.56938900
O	0.24269600	-3.48740200	-2.24877800
O	0.22661100	5.75033400	-0.30776900
O	6.97757400	-2.72011300	-0.52185200
O	-2.96349200	2.19769300	-0.18074100
H	-8.48955000	-1.36269900	-0.00309700
H	0.60158300	-4.36424600	-2.07793500
H	1.17941600	5.87171700	-0.23703300
H	0.18631900	-4.28419000	2.49138300
H	6.79810200	-3.43963300	0.09242000
O	3.67268400	2.40793900	1.21422500
O	3.89679200	1.64466700	2.35629600
H	4.78547500	1.27973200	2.21703600

**Cartesian coordinates RAF TS 11a**

C	1.53771100	3.06959900	-0.23403300
C	0.53652100	2.08185300	-0.20477500
C	-0.81659100	2.50425700	-0.22761400
C	-1.05479800	3.88533900	-0.29371000
C	-0.02044400	4.82848600	-0.31736100
C	1.31436500	4.43365400	-0.28942400
C	2.58855500	1.13159800	-0.09416700
C	1.25190500	0.82022300	-0.09540500
H	-2.07954800	4.23426200	-0.37048100
H	2.11884000	5.15594800	-0.31461300
C	3.81843800	0.34960500	-0.01344400
C	5.00334700	0.95380600	0.43756000
C	3.87091600	-1.00425300	-0.39101500
C	6.18753300	0.23285600	0.52658900

H	4.99343300	1.99751800	0.72381300
C	5.05022500	-1.72848400	-0.30316700
H	2.98651700	-1.49345900	-0.77601000
C	6.21466800	-1.11402200	0.16051200
H	7.09107900	0.71925700	0.88249900
H	5.08789400	-2.76882200	-0.60218200
C	0.70650000	-0.55034100	0.10088700
C	0.05090391	-1.17376638	-0.99189237
C	0.79825665	-1.20145418	1.30296176
C	-0.52970783	-2.46042340	-0.85074743
H	-0.01718755	-0.67256518	-1.94836664
C	0.22329065	-2.57113418	1.52208136
H	1.24526808	-0.72972220	2.17075278
C	-0.48248570	-3.13697881	0.32888211
H	-0.88822674	-4.13525796	0.44130029
C	-1.93095000	1.55520200	-0.21568400
H	-1.71711300	0.57809100	-0.63176800
C	-3.16086500	1.78542200	0.28154900
H	-3.34632200	2.71454700	0.81597200
C	-4.29159000	0.85594000	0.22157800
C	-4.42313400	-0.11586200	-0.78366200
C	-5.30384200	0.91768800	1.19560000
C	-5.48512600	-1.01245200	-0.79252000
H	-3.70804600	-0.14242100	-1.59920900
C	-6.36950900	0.02912500	1.19909000
H	-5.24108500	1.66880200	1.97612900
C	-6.45846400	-0.94924100	0.20733900
H	-5.56583400	-1.75027100	-1.58532800
H	-7.13806600	0.07690800	1.96098500
O	7.34717700	-1.87636000	0.22656200
O	1.19703338	-3.52097092	1.95362733
O	-1.11860738	-2.95559381	-1.98554085
O	-0.26998000	6.17406400	-0.38995200
O	-7.52625800	-1.80145400	0.25410500
O	2.77128000	2.49905900	-0.17725300
H	8.08255500	-1.34309900	0.54643200
H	-1.45012687	-3.84432359	-1.81755200
H	-1.22034700	6.32728600	-0.39874500
H	2.07512628	-3.13786548	1.86052252

**Cartesian coordinates RAF TS 8b**

C	1.68559700	2.74021400	-0.20727200
C	0.70439300	1.74479200	-0.05742100
C	-0.64484700	2.14997600	0.04826000
C	-0.91368900	3.52258600	-0.00469800
C	0.10018100	4.47697900	-0.15533200
C	1.43620500	4.09946500	-0.26300900
C	2.75729500	0.80541500	-0.19406700
C	1.43005000	0.48826000	-0.05362500
H	-1.93591300	3.86268900	0.12427500
H	2.22308100	4.83367300	-0.37047500
C	3.99675400	0.03691700	-0.26092800
C	5.23160000	0.68639300	-0.09758900
C	4.01099300	-1.35014600	-0.49660200
C	6.42802500	-0.01815000	-0.15509200
H	5.25218500	1.75360800	0.07889100
C	5.20220600	-2.05759400	-0.55450400
H	3.08232500	-1.88212700	-0.64751900
C	6.41835400	-1.39503600	-0.38105100
H	7.37012300	0.50585500	-0.02201300
H	5.20654900	-3.12471900	-0.74047500
C	0.85960400	-0.87573600	0.09442000
C	0.90246800	-1.51707600	1.33507500
C	0.28492400	-1.51540900	-1.00957200
C	0.38118100	-2.80367600	1.46293800
H	1.33573800	-1.03167500	2.19950500
C	-0.23341500	-2.80069200	-0.86727000
H	0.24551700	-1.03243800	-1.97739300
C	-0.18830100	-3.45473900	0.36628000
H	-0.58756800	-4.46077400	0.47053400
C	-1.74431500	1.18732400	0.24645000
H	-1.44325700	0.20225900	0.57295400
C	-2.95166100	1.31394000	-0.44050400
H	-3.13363200	2.24378800	-0.97054700
C	-4.02055800	0.35327600	-0.48178900

C -3.97967100 -0.89787100 0.17656400  
 C -5.19026000 0.65331800 -1.22206000  
 C -5.04297900 -1.78399500 0.10016800  
 H -3.11314700 -1.17133800 0.76341100  
 C -6.25277900 -0.22799000 -1.30460800  
 H -5.25124600 1.60440900 -1.74049600  
 C -6.18442900 -1.45604200 -0.63927700  
 H -4.99114900 -2.73693300 0.61944200  
 H -7.14177100 0.01292700 -1.87470200  
 O 7.56157400 -2.14341400 -0.44729100  
 O -0.77265900 -3.38544700 -1.98045100  
 O 0.45703300 -3.38962300 2.69563800  
 O -0.17211500 5.82031000 -0.19132500  
 O -7.25932600 -2.29100000 -0.74616100  
 O 2.92099600 2.17779000 -0.28663000  
 H 8.32949200 -1.57756400 -0.31517800  
 H 0.06777800 -4.26967400 2.66891600  
 H -1.11514700 5.96153300 -0.05938500  
 H -1.08750300 -4.27042500 -1.76979300  
 H -7.10232500 -3.09484000 -0.23935000  
 O -2.21178400 1.73544000 2.06845400  
 O -2.93133600 0.72594100 2.71811400  
 H -3.84675800 1.04356200 2.68329800

**Cartesian coordinates RAF TS 7a**

C -1.42473100 2.69544400 -0.14945000  
 C -0.39902500 1.71580300 -0.17508300  
 C 0.95412700 2.15234000 -0.30666400  
 C 1.15923800 3.53384300 -0.43589000  
 C 0.10850200 4.45674600 -0.40542400  
 C -1.22280400 4.05049300 -0.25279200  
 C -2.43999200 0.75886100 0.19100700  
 C -1.05569000 0.46547100 -0.01530700  
 H 2.16639700 3.90645200 -0.58998900  
 H -2.03124700 4.76760000 -0.22139300  
 C -3.62202600 -0.07232500 -0.10158900  
 C -4.75176400 0.50268200 -0.69697300  
 C -3.66549700 -1.43861000 0.22289900  
 C -5.87936300 -0.26174000 -0.98092600  
 H -4.74759400 1.55620900 -0.94133700

C -4.78618900 -2.20596100 -0.05864900  
 H -2.82021400 -1.90197100 0.71261000  
 C -5.89894900 -1.61987500 -0.66630000  
 H -6.74384600 0.20333700 -1.44571700  
 H -4.81785000 -3.25912000 0.19284600  
 C -0.45763600 -0.89079200 0.02276300  
 C -0.16599400 -1.55469300 -1.17370600  
 C -0.18976400 -1.49728000 1.25348800  
 C 0.39199800 -2.83078600 -1.13047100  
 H -0.37775200 -1.10085400 -2.13321000  
 C 0.37270900 -2.77232500 1.27840900  
 H -0.42447100 -0.99314200 2.18168300  
 C 0.66655900 -3.44774100 0.09129600  
 H 1.09986100 -4.44466700 0.11857200  
 C 2.06431800 1.20599000 -0.30598500  
 H 1.80053700 0.17538300 -0.50603200  
 C 3.35484200 1.50734400 -0.05002400  
 H 3.60665100 2.52579500 0.23553000  
 C 4.49222800 0.59052400 -0.07247800  
 C 4.42301300 -0.72138900 -0.57344000  
 C 5.73518000 1.02603600 0.42307100  
 C 5.53281900 -1.55481900 -0.56659400  
 H 3.49388500 -1.09705300 -0.98492000  
 C 6.85180500 0.20220700 0.43583000  
 H 5.82264200 2.03527700 0.81213000  
 C 6.75330600 -1.09737400 -0.06004300  
 H 5.45585600 -2.56274600 -0.96479700  
 H 7.80225400 0.54900200 0.82271200  
 O -6.97526600 -2.42435200 -0.92023700  
 O 0.61434000 -3.32461300 2.50519300  
 O 0.65519200 -3.44062500 -2.32790800  
 O 0.32516300 5.79863000 -0.53583200  
 O 7.87873500 -1.87411900 -0.03284300  
 O -2.64306700 2.11110200 -0.01050300  
 H -7.67694200 -1.90974200 -1.33295300  
 H 0.98118000 -4.33402400 -2.17813200  
 H 1.26910600 5.97037200 -0.61989900  
 H 1.01922400 -4.19229500 2.40500900  
 H 7.68699900 -2.74027900 -0.40719400

**Cartesian coordinates RAF TS 11b**

C 1.63327200 2.46068300 -0.43848400  
 C 0.61956100 1.47286000 -0.36299600  
 C -0.75447700 1.88115300 -0.49266300  
 C -0.98834400 3.22630500 -0.65344500  
 C 0.05220700 4.23089000 -0.56613200  
 C 1.42208000 3.79989100 -0.59495900  
 C 2.65777300 0.51425900 -0.18411400  
 C 1.29821700 0.22949200 -0.19271600  
 H -1.99790500 3.58159400 -0.82335800  
 H 2.21639500 4.52916500 -0.67032700  
 C 3.86592000 -0.27898800 -0.04285000  
 C 5.12056700 0.31171000 -0.28551500  
 C 3.84190300 -1.63303600 0.34817500  
 C 6.29461100 -0.41650800 -0.15424700  
 H 5.17037900 1.35046000 -0.58318000  
 C 5.01199200 -2.36182600 0.48249300  
 H 2.89999500 -2.11825700 0.55949900  
 C 6.24628200 -1.75852400 0.22927100  
 H 7.25057500 0.05994500 -0.35079000  
 H 4.98800300 -3.40054400 0.78845700  
 C 0.67501600 -1.11320100 -0.05834000  
 C 0.13381500 -1.50477600 1.16853400  
 C 0.62161500 -1.97156800 -1.16070800  
 C -0.45720800 -2.76153900 1.28914600  
 H 0.15854500 -0.84647200 2.02697600  
 C 0.02798200 -3.22525300 -1.02509100  
 H 1.03556800 -1.68128800 -2.11766100  
 C -0.51217900 -3.63037300 0.19703400  
 H -0.97096100 -4.61091600 0.29728100  
 C -1.84925900 0.90407400 -0.50549700  
 H -1.61503900 -0.07194200 -0.91560600  
 C -3.08455400 1.14263500 -0.02859200  
 H -3.26578900 2.09005400 0.47363300  
 C -4.23167800 0.23320700 -0.06711400  
 C -4.28204500 -0.91283200 -0.87775300

C	-5.35468300	0.50675300	0.73369600
C	-5.38932700	-1.75134200	-0.87426200
H	-3.45310400	-1.14760400	-1.53500300
C	-6.46718800	-0.32356500	0.74737500
H	-5.34882900	1.38936700	1.36477200
C	-6.48687300	-1.46095300	-0.05889500
H	-5.40890000	-2.62683100	-1.51759100
H	-7.32517700	-0.10339700	1.37089400
O	7.36503500	-2.52678200	0.37597000
O	0.00050700	-4.02724900	-2.13308500
O	-0.96450700	-3.09714100	2.51194200
O	-0.16397300	5.46096500	-1.13429200
O	-7.60569600	-2.24901200	-0.01957300
O	2.86245000	1.86810600	-0.33837600
H	8.15033400	-2.00470300	0.17965000
H	-1.39063000	-3.95950900	2.47121800
H	-0.99227000	5.81569200	-0.78616500
H	-0.41205500	-4.87085700	-1.92090400
H	-7.50956000	-2.98110000	-0.63748500
O	-0.17584700	4.85059900	1.15947100
O	-0.18089700	3.83418300	2.13358100
H	0.73386800	3.84002700	2.45249100

Cartesian coordinates RAF TS 10b

C	1.48872700	2.55946900	-0.36965400
C	0.57477100	1.49881300	-0.24533700
C	-0.81071000	1.77262500	-0.31239200
C	-1.19509300	3.16484000	-0.37330900
C	-0.19173100	4.19292500	-0.53583100
C	1.15335000	3.90578800	-0.52186100
C	2.70098300	0.72178100	-0.15721100
C	1.39439300	0.30686200	-0.11205900
H	-2.15084000	3.38156100	-0.83594900
H	1.89977300	4.68143500	-0.62690700
C	3.99886900	0.06425900	-0.05905900
C	5.16576400	0.76199900	-0.41419600
C	4.13949000	-1.25926200	0.39856300
C	6.41632700	0.16263600	-0.32916000
H	5.09057100	1.78357500	-0.76226300
C	5.38511100	-1.86138800	0.48501300

H	3.26747400	-1.82180200	0.70057200
C	6.53155900	-1.15393900	0.11874500
H	7.30332200	0.72179700	-0.61258500
H	5.48691000	-2.87894800	0.84205500
C	0.91663000	-1.08946800	0.05688900
C	0.41919500	-1.50573900	1.29568800
C	0.95724800	-1.97967100	-1.02062900
C	-0.02836900	-2.81592800	1.45270200
H	0.37462500	-0.82621100	2.13679600
C	0.50797400	-3.28788600	-0.84862700
H	1.33834800	-1.67195900	-1.98561400
C	0.01390700	-3.71631400	0.38512100
H	-0.33220100	-4.73889600	0.51414600
C	-1.81331600	0.73928500	-0.33660000
H	-1.44548600	-0.26767400	-0.48936900
C	-3.14741100	0.92984300	-0.16499600
H	-3.49703300	1.92620100	0.08651700
C	-4.18516600	-0.08984600	-0.22331300
C	-3.95844800	-1.41358500	-0.64468700
C	-5.49939200	0.24910500	0.15521800
C	-4.98512300	-2.34630300	-0.67592800
H	-2.96924600	-1.71986600	-0.96296700
C	-6.53307600	-0.67510200	0.12956300
H	-5.70551600	1.26248200	0.48308600
C	-6.27834100	-1.98191500	-0.28714900
H	-4.78666800	-3.36025300	-1.01209500
H	-7.53857600	-0.40251700	0.42622300
O	7.73256500	-1.79868400	0.22450800
O	0.57277200	-4.11940200	-1.93338000
O	-0.49598000	-3.17321700	2.68604200
O	-0.60195100	5.47804600	-0.69612700
O	-7.32738200	-2.85916000	-0.30124900
O	2.76113000	2.09996400	-0.32191100
H	8.44468200	-1.20956100	-0.04618500
H	-0.79416700	-4.08854400	2.67652000
H	-1.48757100	5.56036500	-0.30438700
H	0.25817300	-4.99784900	-1.69624000
H	-7.03063200	-3.71845600	-0.61869400
O	-1.88050300	3.50995600	1.34065100

Cartesian coordinates RAF TS 12b

C	1.57715300	2.39060800	-0.41610200
C	0.54425600	1.46508100	-0.34061200
C	-0.81123200	1.93368800	-0.40574100
C	-0.98060200	3.32754600	-0.61451400
C	0.07547100	4.20926100	-0.70025100
C	1.42897600	3.79570300	-0.45821500
C	2.54914700	0.41931500	-0.22717500
C	1.19570100	0.17350400	-0.21724800
H	-1.98324400	3.71919600	-0.74807100
H	2.23536000	4.42019900	-0.82218300
C	3.75255600	-0.40512300	-0.14326400
C	5.00546800	0.20758900	0.02842100
C	3.71661700	-1.80858100	-0.23297400
C	6.16950100	-0.54603600	0.11326400
H	5.06651000	1.28549900	0.09790600
C	4.87582400	-2.56509300	-0.14812100
H	2.77503000	-2.31819200	-0.37807000
C	6.10999400	-1.93754100	0.02667000
H	7.12534100	-0.04827200	0.24858700
H	4.84071500	-3.64528800	-0.22070600
C	0.54821200	-1.16011700	-0.10262100
C	0.33890500	-1.72715600	1.15711100
C	0.15573600	-1.84689200	-1.25668200
C	-0.25420000	-2.98494500	1.25760800
H	0.63568300	-1.20876200	2.05936900
C	-0.43531800	-3.10379100	-1.14235100
H	0.31418800	-1.42299000	-2.23988600
C	-0.64484200	-3.68201000	0.11214100
H	-1.10137100	-4.66524400	0.19547600
C	-1.92688300	1.03171700	-0.27907000
H	-1.67233200	-0.01953300	-0.24777500
C	-3.23771700	1.37758900	-0.17330400
H	-3.50185400	2.43109400	-0.14771300
C	-4.37457900	0.47612900	-0.06102200
C	-4.27502000	-0.92574800	-0.14834300
C	-5.65977400	1.01695600	0.14465900

C	-5.39434100	-1.73644800	-0.02844900	C	-6.83585400	-0.89808000	-0.01036900	H	7.52414500	1.47182000	1.09912000
H	-3.31253700	-1.39326900	-0.31716500	H	-7.58401000	1.07412900	0.43642600				
C	-6.78540900	0.21632100	0.26535800	H	-5.81276200	-2.72351400	-0.46927600				
H	-5.77148900	2.09407500	0.21377900	C	-1.22730800	-0.89151000	-0.00438600				
C	-6.65627700	-1.17015500	0.17993600	C	-0.83080400	-1.51929800	-1.18952100				
H	-5.29169600	-2.81562100	-0.10121200	C	-1.19343200	-1.58922300	1.20643800				
H	-7.76676500	0.64610200	0.42505300	C	-0.40827400	-2.84679300	-1.15727000				
O	7.21917300	-2.73333600	0.10326400	H	-0.85087300	-0.99271900	-2.13481000				
O	-0.79122900	-3.73570200	-2.30196900	C	-0.77061200	-2.91767300	1.22411200				
O	-0.42843000	-3.49380700	2.51374900	H	-1.49878600	-1.11745300	2.13124100				
O	-0.07839800	5.53441300	-0.96752600	C	-0.37512900	-3.55550100	0.04638300				
O	-7.79179300	-1.92151100	0.30246400	H	-0.04898300	-4.59252400	0.06467600				
O	2.78365000	1.77335900	-0.34172400	C	1.53056900	0.92271800	0.00112600				
H	8.00456400	-2.18843900	0.22036100	H	1.15138900	-0.05330600	0.27491600				
H	-0.83925900	-4.36329500	2.46750600	C	2.85586700	1.05095100	-0.28496600				
H	-1.01540500	5.75553000	-1.00457900	H	3.22460700	2.01330300	-0.62584400				
H	-1.15352700	-4.60639500	-2.10809400	C	3.85899200	0.02706000	-0.20078100				
H	-7.57620500	-2.85651200	0.22190400	C	3.63549000	-1.26244800	0.31566500				
O	1.78059000	4.42880800	1.28502700	C	5.21377600	0.37011100	-0.59265300				
O	0.92186400	3.83422000	2.22247700	C	4.64218100	-2.20737700	0.35342900				
H	1.42093400	3.06033400	2.52475400	H	2.65469800	-1.53197600	0.68835900				

### Cartesian coordinates RAF TS 2b

C	-1.74816100	2.79186400	-0.05850400	C	6.20303600	-0.66256900	-0.66455200	H	5.32818600	1.20063200	-1.27935000
C	-0.84991600	1.71012700	-0.04387700	H	5.32818600	1.20063200	-1.27935000	C	5.93258300	-1.90619200	-0.15715500
C	0.54363500	1.98815500	-0.04246500	H	4.44722600	-3.19260300	0.76728500	H	4.44722600	-3.19260300	0.76728500
C	0.91932300	3.34532800	-0.06053300	H	7.18079500	-0.44930600	-1.07760500	H	7.18079500	-0.44930600	-1.07760500
C	-0.01452800	4.38282400	-0.08267500	O	-8.04383400	-1.53814000	-0.01389700	O	-8.04383400	-1.53814000	-0.01389700
C	-1.38709400	4.12491700	-0.08181200	O	-0.76188600	-3.55470600	2.43412000	O	-0.76188600	-3.55470600	2.43412000
C	-2.98522800	0.95925200	-0.03612300	O	-0.03943000	-3.41440600	-2.34475900	O	-0.03943000	-3.41440600	-2.34475900
C	-1.68238100	0.52327100	-0.03219000	O	0.36316700	5.69920400	-0.08902900	O	0.36316700	5.69920400	-0.08902900
H	1.97219700	3.60202000	-0.01615400	O	6.92382800	-2.85053000	-0.17061500	O	6.92382800	-2.85053000	-0.17061500
H	-2.11148400	4.92787700	-0.08802100	O	-3.03128700	2.34211300	-0.04985700	O	-3.03128700	2.34211300	-0.04985700
C	-4.28966500	0.30551300	-0.02818700	H	-8.74828700	-0.90801800	0.17098700	H	-8.74828700	-0.90801800	0.17098700
C	-5.44749400	1.06081600	0.22451000	H	0.23774200	-4.32586800	-2.20591000	H	0.23774200	-4.32586800	-2.20591000
C	-4.44631200	-1.07035400	-0.27935600	H	1.32396000	5.76197000	-0.07351400	H	1.32396000	5.76197000	-0.07351400
C	-6.70451400	0.46929100	0.23554400	H	-0.47989000	-4.46890100	2.32621300	H	-0.47989000	-4.46890100	2.32621300
H	-5.35937100	2.12200600	0.41532000	H	6.57950600	-3.69093400	0.14826500	H	6.57950600	-3.69093400	0.14826500
C	-5.69869400	-1.66487700	-0.27034600	O	5.65820500	1.43523300	0.85972300	O	5.65820500	1.43523300	0.85972300
H	-3.58258000	-1.68314700	-0.49453800	O	6.90777000	2.04556900	0.61997600	O	6.90777000	2.04556900	0.61997600