Supplementary Information

Benzylperoxy radical cation: an exceptionally stable and bound species

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Computational method

Geometry optimizations of local minima and transition state (TS) structures were carried out using density functional theory (DFT) with the M06 and B3LYP functional, with 6-311++G(2df,p) basis sets. The TSs were confirmed by attaining one imaginary mode in the vibrational frequency calculations at the same level. The intrinsic reaction coordinate (IRC) calculations were performed at a similar level of theory to confirm the connectivity between intermediate (INT) and TS structures in the reaction. To facilitate IBO transformation, the optimization of TS structure and IRC calculations are repeated with the B3LYP/aug-cc-pVTZ basis sets.[1-3] The single-point energy calculations were performed with the explicitly correlated coupled cluster method with single, double, and perturbative triple excitations at the CCSD(T)-F12(b)/cc-pVQZ-F12 level,[4-7] and all energies were corrected with the zero-point vibrational energy (ZPVE) corrections at the B3LYP/6-311++G(2df,p) level. For stable structures core−valence correlation (CV) at the CCSD(T)/cc-pwCVTZ level was also included.[8] In the IBO analysis, the orbital change for an orbital *i*, is defined as

$$\Delta_i(s) = \sqrt{\sum_{A=1}^{atoms} \left(n_{A,i}(s) - n_{A,i}(0)\right)^2}$$

where A sums over the atoms involved in i and $n_{A,i}(s)$ measures the number of electrons on atom A at IRC arc length s. Effectively, $\Delta_i(s)$ quantifies the deviation of charge on the involved atoms with respect to the initial charge distribution at s = 0.

All the DFT (default grid size) geometry optimizations and vibrational frequency calculations, and NBO analysis were done using the Gaussian 16 package of programs and affiliated NBO 7.0 program. The CCSD(T) and CCSD(T)-F12 calculation were performed using the MOLPRO 2022 program suite.[9] The IBO analysis were done with the IboView program obtained at http://www.iboview.org/.

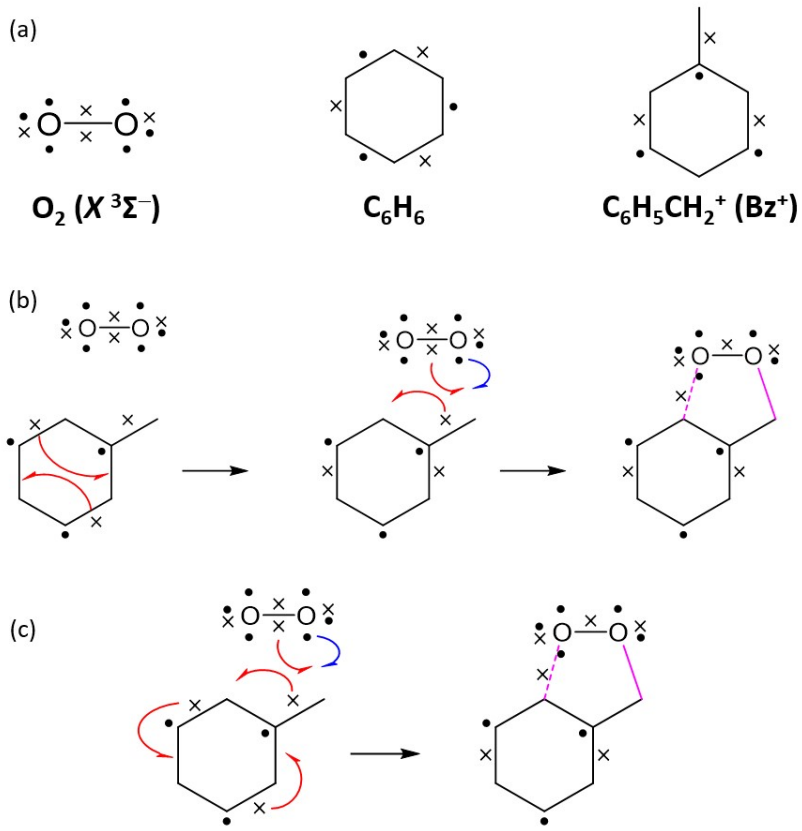

Figure S1. The Linnett structure of a) $O_2(^3\Sigma^-)$, C_6H_6 and $C_6H_5CH_2^+(Bz^+)$ according to the Linnett double-quartet theory. b) The speculated mechanism of O_2 addition to Bz^+, the curly arrows in Linnett structures (cross and dot represents α and β electrons, respectively) are drawn in accordance with the electron flow revealed by IBO analysis. c) The alternative single-step mechanism of O_2 addition to Bz^+, this version is to conceal the long-distant flow of aromatic electrons. This compact yet intuitive mechanism cannot be derived by starting from conventional valence bond picture; the charge and spin densities cannot never be rationalized despite forcible attempts.

Table S1. The natural bond orbital analysis on the orbital interactions in the $C_2H_5OO^+$ and $C_6H_5CH_2OO^+$ cations (triplet state) at the B3LYP/6-311++G(2df,p) level.[a]

	Interactions	$E(2)$ [b]	ΔE [c]	F [d]	$r(C_\alpha–O)$ in cation – $r(C_\alpha–O)$ in neutral [e]
$C_2H_5OO^+$ [f]	$\sigma(C_\beta–H)\rightarrow\sigma^*(C_\alpha–O)$	17.7	200.8	60.3	0.72
	$\sigma(C_\beta–H')\rightarrow\sigma^*(C_\alpha–O)$	1.1	213.4	15.1	
$BzOO^+$	**α:** $\pi(C_\delta–C_\varepsilon)\rightarrow\sigma^*(C_\gamma–O')$	41.4	81.6	57.7	0.018
	α: $\pi(C_\beta–C_\gamma')\rightarrow\sigma^*(C_\gamma–O')$	32.8	87.9	54.0	
	α: $\pi(C_\beta–C_\gamma')\rightarrow\sigma^*(C_\alpha–O)$	3.9	282.4	33.3	
	β: $\pi(C_\delta–C_\varepsilon)\rightarrow\sigma^*(C_\gamma–O')$	19.5	106.7	45.2	
	β: $\pi(C_\beta–C_\gamma')\rightarrow\sigma^*(C_\gamma–O')$	12.9	113.0	38.3	
	β: $\pi(C_\beta–C_\gamma')\rightarrow\sigma^*(C_\alpha–O)$	3.1	282.4	30.1	
TS [$BzOO^+(X^3A)\rightarrow Bz^+ + O_2(^3\Sigma^-)$]	**α:** $\pi(C_\delta–C_\varepsilon)\rightarrow\sigma^*(C_\gamma–O')$	37.7	87.9	58.4	---
	α: $\pi(C_\beta–C_\gamma')\rightarrow\sigma^*(C_\gamma–O')$	30.7	100.4	54.6	
	α: $\pi(C_\beta–C_\gamma')\rightarrow\sigma^*(C_\alpha–O)$	5.0	251.0	35.1	
	β: $\pi(C_\delta–C_\varepsilon)\rightarrow\sigma^*(C_\gamma–O')$	15.6	75.3	33.9	
	β: $\pi(C_\beta–C_\gamma')\rightarrow\sigma^*(C_\gamma–O')$	34.1	87.9	54.6	
	β: $\pi(C_\beta–C_\gamma')\rightarrow\sigma^*(C_\alpha–O)$	7.0	244.7	41.4	

[a] The unit of $E(2)$, ΔE and F is in kcal/mol. H and H' are the on-the-plane and out-of-plane alkyl hydrogen atoms, respectively. O and O′ are the alkyl (or benzyl) oxygen and the terminal oxygen, respectively.
[b] The stabilization energy, $E(2)$, is defined as $F^2/\Delta E$.
[c] The orbital energy difference, ΔE, is the energy between acceptor and donor orbitals.
[d] F is the off-diagonal NBO Fock matrix element.
[e] The change of optimized $C_\alpha–O$ bond length (in Å) from ROO (triplet) to ROO^+, where R = C_2H_5 (ref. 38) and Bz (this work, B3LYP value, Figure 1).
[f] The interactions found in the α and β electron spins are very similar, only the values of α spin are given.

Table S2. Cartesian coordinates for the optimized geometries at B3LYP/6-311++G(2df,p) level.

BzOO ($X\,^2A''$)

O	1.16881800	3.33281100	0.00000000
O	1.07797400	2.02345800	0.00000000
C	-0.32842200	1.58079000	0.00000000
C	-0.35166900	0.08578900	0.00000000
C	-0.35171800	-0.62134500	1.20258200
C	-0.35171800	-0.62134500	-1.20258200
C	-0.35171800	-2.01047000	1.20399300
C	-0.35171800	-2.01047000	-1.20399300
H	-0.35191200	-0.07987900	2.14199200
H	-0.35191200	-0.07987900	-2.14199200
H	-0.35396400	-2.54964400	2.14350000
H	-0.35396400	-2.54964400	-2.14350000
H	-0.78669200	2.01040100	0.89087900
H	-0.78669200	2.01040100	-0.89087900
C	-0.35211900	-2.70660200	0.00000000
H	-0.35471800	-3.78997600	0.00000000

$BzOO^+$ ($X\,^3A$)

C	-1.45895100	-1.31980000	0.26972900
C	-0.17262100	-0.84620100	0.62272900
C	0.19520000	0.50661900	0.38218900
C	-0.74539000	1.38528900	-0.08796100
C	-2.05195000	0.92194000	-0.36741100
C	-2.39699100	-0.43235000	-0.20181100
H	-1.70523200	-2.36146000	0.42933900
H	0.47966900	-1.49111100	1.19890900
H	-0.49282900	2.41853900	-0.29131100
H	-2.78444000	1.61631000	-0.76127100
H	-3.40075100	-0.76247000	-0.43591100
C	1.63566000	0.87421800	0.54150900
H	2.03086000	0.71317800	1.54723900
H	1.88323000	1.87756800	0.20180900
O	2.44559000	-0.01705200	-0.34330100
O	1.79937900	-1.05155200	-0.76203100

$BzOO^+$ ($a\,^1A$)

C	0.29675600	1.04606400	0.37381200
C	1.60266300	1.39513700	0.11383700
C	2.52481500	0.39952800	-0.23228900
C	2.14419200	-0.95200100	-0.30059500
C	0.84264700	-1.31063600	-0.03378100
H	-0.43724100	1.81105200	0.60283100
H	1.91041200	2.43157500	0.15266900
H	3.54364900	0.67730400	-0.47436000
H	2.87596600	-1.70576900	-0.56029800
H	0.53738300	-2.34877100	-0.07801400
C	-0.08135600	-0.31825100	0.35727100
C	-1.46935500	-0.69145000	0.74496200
H	-1.64899300	-1.76294700	0.80941700
H	-1.94019300	-0.12849200	1.54675900
O	-2.13880100	-0.27724900	-0.53746600
O	-2.86159300	0.72921100	-0.47982200

TS: $BzOO^+$ ($X\,^3A$) $\rightarrow$ $Bz^+ + O_2$ ($X\,^3\Sigma^-$)

C	-1.52954600	-1.30781400	0.25146700
C	-0.22613900	-0.88974300	0.62912100
C	0.17012800	0.43289300	0.43483100
C	-0.74222900	1.33752200	-0.08444800
C	-2.07226700	0.92961300	-0.40058800
C	-2.45095600	-0.38885000	-0.25012600
H	-1.81084200	-2.34476600	0.38779600
H	0.42007900	-1.59421800	1.13719100
H	-0.45083600	2.36442500	-0.27264900
H	-2.76572700	1.66155900	-0.79518800
H	-3.44831100	-0.70983000	-0.52007200
C	1.58486100	0.80639800	0.66730400
H	2.01418500	0.43626700	1.59768400
H	1.82332800	1.85533200	0.51713300
O	2.45255400	0.11837000	-0.41116400
O	2.02432200	-1.01698000	-0.78099300

Table S3. Cartesian coordinates for the optimized geometries at CCSD(T)/6-311+G(d) level.

BzOO ($X\,^2A''$)

C	-0.13514219	2.04387661	1.21661922

C	-0.13514219	2.04387661	-1.21661922
C	0.20474257	0.68194637	1.21532375
C	0.20474257	0.68194637	-1.21532375
C	0.37808926	-0.00636934	0.00000000
C	-0.30543154	2.72585564	0.00000000
H	-0.26511855	2.57109053	2.16245296
H	-0.26511855	2.57109053	-2.16245296
H	0.33465439	0.15126660	2.16087972
H	0.33465439	0.15126660	-2.16087972
H	-0.56738912	3.78464814	0.00000000
C	0.70082488	-1.47412003	0.00000000
H	1.24699120	-1.78789037	0.89769068
H	1.24699120	-1.78789037	-0.89769068
O	-0.57719370	-2.20103682	0.00000000
O	-0.36868631	-3.50722074	0.00000000

$BzOO^+$ ($X\,^3A$)

C	-1.15720151	-1.43022418	0.03957603
C	0.12188820	-0.97138757	0.50037685
C	0.49837656	0.41168171	0.34935212
C	-0.41796285	1.32771746	-0.12997279
C	-1.72402466	0.87704718	-0.49171595
C	-2.07488861	-0.50136828	-0.43005366
H	-1.41435553	-2.48465345	0.13142548
H	0.69560610	-1.61490758	1.17063346
H	-0.14687610	2.37296702	-0.28064045
H	-2.44578558	1.59694366	-0.87891278
H	-3.07266551	-0.81588139	-0.73359164
C	1.96783112	0.67258121	0.47647373
H	2.39378828	0.40953971	1.45307842
H	2.28814825	1.67067766	0.16632995
O	2.62336212	-0.25405590	-0.51196729
O	1.86475975	-1.26667725	-0.83039147

$BzOO^+$ ($a\,^1A$)

C	0.26558245	1.04668350	0.34493598
C	1.58725963	1.40806269	0.11408399
C	2.52680431	0.40638492	-0.23122847
C	2.15781617	-0.96482595	-0.29167183
C	0.84204891	-1.33692516	-0.04723040
H	-0.49142846	1.81031490	0.54313370
H	1.88551490	2.45525161	0.13427396
H	3.55259440	0.69312369	-0.46674229
H	2.90227321	-1.71609699	-0.55262054
H	0.54141764	-2.38460159	-0.08589620
C	-0.09192693	-0.33862466	0.36352537
C	-1.48991608	-0.71122865	0.75327021
H	-1.67166225	-1.78887279	0.80176529
H	-1.94807041	-0.15436287	1.57486189
O	-2.09750657	-0.25535637	-0.51802286
O	-2.77005093	0.82491774	-0.43196481

TS: $BzOO^+$ ($X\,^3A$) $\rightarrow$ $Bz^+ + O_2$ ($X\,^3\Sigma^-$)

C	0.20039500	0.53133200	0.52584300
C	1.61146100	0.90720900	0.64872800
C	-0.12248100	-0.82521900	0.73510900
C	-0.72755800	1.37766100	-0.09629400

C	-2.04566300	0.90522600	-0.42602500
C	-1.39843700	-1.31011000	0.32900000
C	-2.35458400	-0.43563800	-0.26019900
O	2.33442700	-0.00309600	-0.54700500
O	1.74488100	-1.08479900	-0.78564000
H	2.16259400	0.53359600	1.51552500
H	1.90101900	1.91584600	0.34981500
H	-0.45523500	2.40648500	-0.34040900
H	-2.76305100	1.59426700	-0.87008700
H	-3.32807500	-0.82225200	-0.55818800
H	-1.64709600	-2.36011700	0.48538000
H	0.51658200	-1.46743600	1.34214500

Table S4. The IRC and IBO results corresponding to Figure 5. All energy is relative to fully optimized energy of $BzOO^+$ at B3LYP/aug-cc-pVTZ level. IBO changes are measured and plotted as the root-mean-square deviation for the orbital partial charge distribution among the atoms with respect to the initial partial charge distribution. Structures [I-V] and [TS] with IBOs presented in Figure 4 are in boldface.

Step number[a]	IRC / bohr amu$^{1/2}$	relative energy / kJ mol^{-1}	orbital change / e^{-1}					
			IBO-1α	IBO-2α	IBO-1β	IBO-2β	IBO-3β	IBO-4β
-50	-15.0	-102						
-49	-14.7	-102						
-48	-14.4	-102						
-47	-14.1	-102						
-46	-13.8	-102						
-45	-13.6	-102						
-44	-13.3	-102						
-43	-13.0	-102						
-42	-12.7	-102						
-41	-12.5	-102						
-40	-12.2	-102	0.00	0.00	0.00	0.00	0.00	0.00
-39	-11.9	-102						
-38	-11.6	-102						
-37	-11.3	-102						
-36	-11.0	-102						
-35	-10.7	-101						
-34	-10.4	-101						
-33	-10.1	-101						
-32	-9.83	-101						
-31	-9.53	-100						
-30	-9.24	-99.9						
-29	-8.95	-99.3						
-28	-8.66	-98.9						
-27	-8.36	-98.4						
-26	-8.06	-97.7						
-25	-7.75	-96.8						
-24	-7.44	-95.8						
-23	-7.13	-94.6						
-22	-6.82	-93.2						
-21	-6.51	-91.6						
-20	-6.20	-89.8						

-19	-5.89	-87.7						
-18	-5.58	-85.3						
-17	-5.28	-82.5						
-16	-4.97	-79.5						
-15 [I]	**-4.66**	**-76.0**	**0.060**	**0.059**	**0.012**	**0.015**	**0.033**	**0.023**
-14	-4.35	-72.1						
-13	-4.04	-67.6						
-12	-3.73	-62.6						
-11	-3.42	-57.0						
-10	-3.11	-51.0	0.123	0.129	0.023	0.035	0.066	0.042
-9	-2.80	-44.3						
-8	-2.48	-37.2						
-7	-2.17	-29.8						
-6 [II]	**-1.86**	**-22.3**	**0.228**	**0.226**	**0.040**	**0.095**	**0.141**	**0.084**
-5	-1.55	-15.1	0.264	0.253	0.049	0.127	0.181	0.109
-4 [III]	**-1.24**	**-8.66**	**0.301**	**0.276**	**0.076**	**0.171**	**0.240**	**0.159**
-3	-0.93	-3.37	0.338	0.297	0.543	0.754	0.507	0.228
-2 [IV]	**-0.62**	**0.36**	**0.371**	**0.322**	**0.557**	**0.815**	**0.629**	**0.330**
-1	-0.31	2.29	0.396	0.347	0.572	0.854	0.705	0.425
0 [TS]	**0.00**	**2.82**	**0.415**	**0.357**	**0.586**	**0.879**	**0.756**	**0.515**
1	0.31	2.58						
2	0.61	2.07	0.434	0.358	0.599	0.904	0.797	0.614
3	0.92	1.61						
4	1.22	1.79						
5	1.50	1.33	0.431	0.351	0.598	0.892	0.802	0.626
6	1.77	0.81						
7	2.06	0.40						
8	2.35	0.16						
9 [V]	**2.65**	**0.06**	**0.441**	**0.350**	**0.606**	**0.907**	**0.818**	**0.672**

[a] The step number is defined as 0 at the TS structure, negative toward the dissociated pair $Bz^+ + O_2$, and positive toward the adduct $BzOO^+$.

Table S5. Cartesian coordinates for geometries selected for IBO change calculations along the IRC pathway computed at the B3LYP/aug-cc-pVTZ level.

Step# -40

C	-1.64282000	-1.22656700	0.52080300
C	-0.49521000	-0.70080000	1.04989400
C	-0.12065900	0.65289800	0.74605000
C	-0.96051000	1.44074200	-0.11154200
C	-2.10633700	0.89499600	-0.63641600
C	-2.44183000	-0.43081400	-0.31619200
H	-1.93932500	-2.24140500	0.74317100
H	0.13864000	-1.28718700	1.70260400
H	-0.67303300	2.45907800	-0.33683700
H	-2.74765700	1.47451100	-1.27860900
H	-3.34732500	-0.85475900	-0.73342100
C	1.02478000	1.18453900	1.26402900
H	1.67007800	0.61138300	1.91827300
H	1.32276600	2.20252700	1.04532500
O	2.93911100	-0.21084600	-0.93190400
O	2.47076700	-1.29979500	-1.14900500

Step# -15; **structure [I]**

C	-1.56066700	-1.27164100	0.41719100
C	-0.32382000	-0.82075300	0.79586800
C	0.05977200	0.52506000	0.50485700
C	-0.84185700	1.38135500	-0.20000600
C	-2.10005000	0.93478700	-0.51305300
C	-2.45401600	-0.38529700	-0.20928800
H	-1.86545800	-2.28803900	0.61994500
H	0.36624600	-1.46900700	1.31821300
H	-0.53259200	2.38958400	-0.44121100
H	-2.81010800	1.58400400	-1.00452200
H	-3.44390300	-0.73714900	-0.46948900
C	1.27251500	1.01552100	0.91980600
H	1.90537300	0.46179700	1.58741000
H	1.58259100	2.02332600	0.67456200
O	2.58676500	-0.02074500	-0.63859200
O	2.17805400	-1.13764000	-0.79231900

Step# -10

C	-1.54946700	-1.27383900	0.40360400
C	-0.30319900	-0.83379600	0.76462000
C	0.08870700	0.50170800	0.46758000
C	-0.82127900	1.36687600	-0.20425800
C	-2.09532000	0.93708900	-0.48908300
C	-2.45319400	-0.38280200	-0.20420800
H	-1.85284500	-2.29114500	0.60375900
H	0.38746700	-1.49596000	1.26924600
H	-0.51031000	2.37388000	-0.44758000
H	-2.80822600	1.60360700	-0.95166300
H	-3.44610100	-0.73103300	-0.45760600
C	1.34299800	0.97078800	0.82012600
H	1.94825300	0.46093000	1.55896900
H	1.66972700	1.96214500	0.53220800
O	2.50191600	0.01828200	-0.55263500
O	2.13313100	-1.10171600	-0.74930400

Step# -6; **structure [II]**

C	-1.54125600	-1.27029300	0.39634100
C	-0.28558800	-0.83786600	0.74426100
C	0.10801400	0.48530300	0.44864700
C	-0.81454200	1.35375600	-0.19917100
C	-2.10078000	0.93474300	-0.47767500
C	-2.46085500	-0.38112400	-0.20814200
H	-1.84211500	-2.28807200	0.60004400
H	0.39901000	-1.51262400	1.23936900
H	-0.50413800	2.35917300	-0.45184900
H	-2.80641300	1.61271500	-0.93447800
H	-3.44876400	-0.73719500	-0.46782900
C	1.42155300	0.92410700	0.73317700
H	1.96718600	0.48476300	1.56075100
H	1.72630700	1.92647400	0.45892300
O	2.44552800	0.05413700	-0.48457000
O	2.09501900	-1.07716100	-0.72018000

Step# -5

C	-1.54008600	-1.26880200	0.39298600
C	-0.28057600	-0.83810000	0.73965500
C	0.11220700	0.48223200	0.44501900
C	-0.81282300	1.34974300	-0.19637400
C	-2.10360900	0.93319500	-0.47543800
C	-2.46468900	-0.38201800	-0.20953800
H	-1.83969900	-2.28581200	0.60128400
H	0.40069100	-1.51477000	1.23688300
H	-0.50320500	2.35336700	-0.45659400
H	-2.80616500	1.61401700	-0.93398500
H	-3.45124800	-0.73879100	-0.47119100
C	1.44457800	0.91246100	0.71141700
H	1.96924300	0.49167200	1.56333300
H	1.73442200	1.92204900	0.45041700
O	2.43616700	0.06523600	-0.46831700
O	2.08221400	-1.07309900	-0.71321100

Step# -4; **structure [III]**

C	-1.53834800	-1.26770800	0.38911900
C	-0.27392500	-0.83488000	0.73437700
C	0.11703400	0.47624300	0.44362000
C	-0.81131900	1.34530800	-0.19329100
C	-2.10826000	0.92787200	-0.47262000
C	-2.47053400	-0.37934300	-0.21298000
H	-1.83687600	-2.28514100	0.59875100
H	0.40154900	-1.51226600	1.23788800
H	-0.50124100	2.34723000	-0.46010700
H	-2.80766200	1.61287200	-0.92928800
H	-3.45617900	-0.73889300	-0.47439000
C	1.46717700	0.90195000	0.69080200
H	1.97362000	0.50832800	1.56722100
H	1.74537500	1.91721300	0.43694700
O	2.42855500	0.07441400	-0.45289800
O	2.06878500	-1.06830100	-0.70627200

Step# -3

C	-1.54144300	-1.26704800	0.38290400
C	-0.26714400	-0.83090100	0.72906000
C	0.12094900	0.47399900	0.44015300
C	-0.80542100	1.34145300	-0.18826000
C	-2.11247600	0.92110000	-0.46990700
C	-2.47571500	-0.38089200	-0.21478400
H	-1.83600600	-2.28535500	0.59494100
H	0.40153900	-1.50770500	1.24229300
H	-0.49860400	2.34313200	-0.46048700
H	-2.80903600	1.61074200	-0.92454300
H	-3.46179600	-0.73956000	-0.47405500
C	1.48981900	0.89300100	0.67123300
H	1.97568600	0.52454000	1.57077000
H	1.75382100	1.91437700	0.42685100
O	2.42406900	0.08486300	-0.43810400
O	2.05276600	-1.06538000	-0.69950900

Step# -2; **structure [IV]**

C	-1.54681400	-1.26751200	0.37539400
C	-0.26040900	-0.82582500	0.72298800
C	0.12533400	0.47357900	0.43541000
C	-0.79723800	1.33830400	-0.18256600
C	-2.11584900	0.91275300	-0.46664700
C	-2.48040700	-0.38395000	-0.21588000
H	-1.83493900	-2.28837200	0.58608500
H	0.39937400	-1.49941200	1.25138800
H	-0.49639900	2.34246900	-0.45321900
H	-2.81016000	1.60715700	-0.91713900
H	-3.46796700	-0.74098100	-0.47074500
C	1.51040600	0.88622300	0.65344800
H	1.97780800	0.54766100	1.57445100
H	1.76372600	1.91154800	0.41164600
O	2.42135300	0.09344900	-0.42396800
O	2.03526600	-1.06236000	-0.69287000

Step# -1

C	-1.55289200	-1.27021600	0.36757300
C	-0.25717800	-0.82338700	0.71600100
C	0.12983300	0.47702400	0.42691200
C	-0.78857500	1.33764400	-0.17694300
C	-2.11442800	0.90652300	-0.46286900
C	-2.48265400	-0.39176500	-0.21428000
H	-1.83421300	-2.29299300	0.57850700
H	0.39459400	-1.49094300	1.26148400
H	-0.49532600	2.34485500	-0.44409800
H	-2.80788600	1.60303600	-0.91191000
H	-3.47280600	-0.74383500	-0.46486200
C	1.52912700	0.88157800	0.63731300
H	1.97681200	0.56776400	1.57685400
H	1.77312600	1.91053500	0.39893300
O	2.42058600	0.10081500	-0.41030700
O	2.01468900	-1.05874900	-0.68597900

Step# 0; **structure [TS]**

C	-1.55745200	-1.27593400	0.36076010
C	-0.25726400	-0.82415700	0.70861640
C	0.13360600	0.48213000	0.41550100
C	-0.78107200	1.34032200	-0.17231100
C	-2.10834800	0.90326100	-0.45906320
C	-2.48139500	-0.40218000	-0.21065290
H	-1.83376100	-2.29933000	0.57407120
H	0.38926000	-1.48348100	1.27029370
H	-0.49464200	2.34996000	-0.43623190
H	-2.80318900	1.59854400	-0.90892190
H	-3.47519200	-0.74641400	-0.45706310
C	1.54541500	0.87852900	0.62265670
H	1.97257900	0.58401500	1.57856160
H	1.78111300	1.91098500	0.38913470
O	2.42130000	0.10683400	-0.39703520
O	1.99115800	-1.05419600	-0.67903540

Step# 2

C	-1.55568800	-1.28965700	0.34666400
C	-0.25527200	-0.82686400	0.69396200
C	0.14053200	0.49151100	0.39550300
C	-0.77300100	1.34889600	-0.16487800
C	-2.09584700	0.90012500	-0.45056500
C	-2.47410400	-0.41925000	-0.20450000
H	-1.82304200	-2.31567300	0.55796400
H	0.38391300	-1.46900200	1.28431500
H	-0.49887600	2.36504000	-0.41530500
H	-2.79648700	1.59078300	-0.89924800
H	-3.47467600	-0.75164000	-0.44019700
C	1.56562000	0.88373100	0.59977300
H	1.96470000	0.63223100	1.58214800
H	1.79126900	1.91623700	0.35272700
O	2.42570300	0.10564700	-0.37121100
O	1.94200900	-1.04627500	-0.66847900

Step# 5

C	-1.53192000	-1.29848300	0.33690700
C	-0.24324500	-0.82674700	0.68329400
C	0.14289400	0.49945900	0.39098000
C	-0.78095900	1.35978400	-0.16257100
C	-2.09189500	0.90259500	-0.44361700
C	-2.45914500	-0.42429600	-0.20472900
H	-1.78837100	-2.32985800	0.53681400
H	0.40737100	-1.46283600	1.26619700
H	-0.51351000	2.37959700	-0.40701900
H	-2.80373700	1.58616700	-0.88421300
H	-3.45772800	-0.76370900	-0.43712600
C	1.56189200	0.90217200	0.59291500
H	1.95836000	0.69384000	1.58583700
H	1.79270400	1.92285900	0.29646500
O	2.42786800	0.07991200	-0.34929000
O	1.90275300	-1.04370100	-0.66918500

Step# 9; **structure [V]**

C	-1.48777400	-1.31259000	0.30483600
C	-0.21113900	-0.81389300	0.66240000
C	0.14797200	0.53355200	0.37848000
C	-0.79113700	1.38312200	-0.14034100
C	-2.08846800	0.89737100	-0.42440800
C	-2.42472700	-0.45362000	-0.21337500
H	-1.72639200	-2.34846700	0.49683600
H	0.43469600	-1.42939900	1.27404000
H	-0.54513900	2.40887900	-0.37688700
H	-2.81847000	1.56793100	-0.85723800
H	-3.41987100	-0.80052300	-0.45168200
C	1.57876300	0.93227600	0.55399000
H	1.95704200	0.81314400	1.57212700
H	1.81067700	1.92914400	0.18627900
O	2.42539400	0.02934200	-0.28684900
O	1.80465600	-1.03916800	-0.67076100

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