Electronic Supporting Information

Unveiling the Non-polar [3+2] Cycloaddition Reactions of Cyclic Nitrones with Strained Alkylidene Cyclopropanes within the Molecular Electron Density Theory Study

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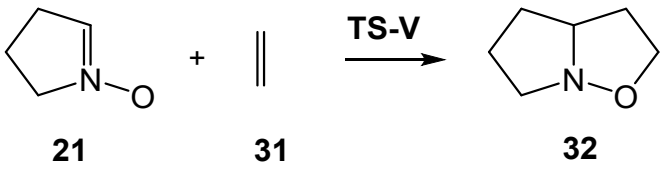
*S1. Non-polar zw-type 32CA reaction of cyclic nitrone **21** with ethylene **31**.*



Scheme S1. 32CA reaction of cyclic nitrone **21** with ethylene **31**

Table S1. *ω*B97X-D/6-311G(d,p) total energies, E in au, and relative energies, ΔE in kcal·mol^{-1}, in gas phase, *, and in benzene, **, and thermodynamic data, computed at 80 ºC in benzene, of the stationary points associated with the 32CA reaction of cyclic nitrone **21** with ethylene **31**.

	E*	ΔE*	E**	ΔE**	H	ΔH	S	ΔS	G	ΔG
21	-286.520814		-286.525684		-286.406394		76.8		-286.449632	
31	-78.579526		-78.580122		-78.524059		56.84		-78.556048	
TS-V	-365.082675	11.1	-365.086066	12.4	-364.909214	13.3	89.8	-43.9	-364.959742	28.8
32	-365.152250	-32.6	-365.155163	-31.0	-364.974406	-27.6	85.3	-48.4	-365.022422	-10.5

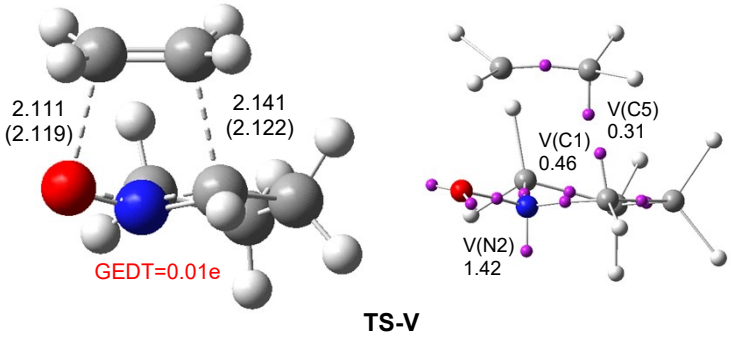


Figure S1. *ω*B97X-D/6-311G(d,p) Gas phase geometries and ELF basin attractor positions together with the most relevant valence basin populations of **TS-V** involved in the 32CA reaction of cyclic nitrone **21** with ethylene **31**. The lengths are given in angstroms and valence basin populations are given in average number of electrons, e. Distances in benzene are given in parentheses.

*S2. Comparative analyses of the MPWB1K, ωB97X-D and PBE0 functionals towards the CCSD(T)/cc-pVTZ energies in the zw-type 32CA reaction of cyclic nitrone **21** with MCP **11**.*

Table S2 Total (E in au) and relative (ΔE in kcal·mol^{-1}) energies computed with the MPWB1K, *ω*B97X-D and PBE0 functional together with the 6-311G(d,p) basis set, and with CCSD(T)/cc-pVTZ level of the stationary points involved in the *zw-type* 32CA reaction of cyclic nitrone **21** with MCP **11**.

	MPWB1K/6-311G(d,p)		*ω*B97X-D/6-311G(d,p)		PBE0/6-311G(d,p)	
	E	ΔE	E	ΔE	E	ΔE
21	-286.461473		-286.520814		-286.115326	
MCP **11**	-155.908921		-155.946963		-155.711143	
TS-II-o	-442.351610	11.8	-442.452502	9.6	-441.804687	13.7
TS-II-m	-442.347242	14.5	-442.449710	11.3	-441.799618	16.8
25	-442.439029	-43.1	-442.534036	-41.6	-441.897813	-44.8
26	-442.435277	-40.7	-442.530187	-39.2	-441.893296	-41.9

	CCSD(T)/cc-pVTZ// MPWB1K/6-311G(d,p)		CCSD(T)/cc-pVTZ// *ω*B97X-D/6-311G(d,p)	
	E	ΔE	E	ΔE
21	-286.064418		-286.066173	
MCP **11**	-155.663281		-155.664132	
TS-II-o	-441.712494	9.5	-441.715037	9.6
TS-II-m	-441.709864	11.2	-441.712560	11.1
25	-441.7913004	-39.9	-441.795242	-40.7
26	-441.7888206	-38.3	-441.791391	-38.3

Table S3. *ω*B97X-D/6-311G(d,p) total energies, E in a.u., and relative energies, ΔE in kcal·mol^{-1}, in gas phase and in benzene, of the stationary points associated with the 32CA reactions of cyclic nitrone **21** with MP **22**, MCP **11** and DCP **27**, and that of cyclic dimethyl nitrone **14** with MCP **11**.

	E	ΔE	E	ΔE
	gas phase		benzene	
21	-286.520814		-286.525684	
22 MP	-157.214265		-157.214928	
TS-I-o	-443.716944	11.4	-443.719918	13.0
TS-I-m	-443.709799	15.9	-443.712889	17.4
23	-443.786847	-32.5	-443.789613	-30.7
24	-443.781391	-29.1	-443.784099	-27.3
11 MCP	-155.946963		-155.947744	
TS-II-o	-442.452502	9.6	-442.455556	11.2
TS-II-m	-442.449710	11.3	-442.452998	12.8
25	-442.534036	-41.6	-442.536888	-39.8
26	-442.530187	-39.2	-442.533269	-37.6
27 DCP	-233.312872		-233.313861	
TS-III	-519.819904	8.6	-519.822987	10.4
28	-519.914949	-51.0	-519.918004	-49.2
14	-365.157507		-365.161639	
TS-IV-o	-521.087967	10.4	-521.090540	11.8
TS-IV-m	-521.085717	11.8	-521.088429	13.1
29	-521.163642	-37.1	-521.166103	-35.6
30	-521.162360	-36.3	-521.165038	-34.9

Table S4. ωB97X-D/6-311G(d,p) enthalpies, H, in a.u., entropies, S in cal·mol^{-1}K^{-1}, and Gibbs free energies, G in a.u., computed at 80 ºC in benzene, for the stationary points associated with the 32CA reactions of cyclic nitrone **21** with MP **22**, MCP **11** and DCP **27**, and that of cyclic dimethyl nitrone **14** with MCP **11**.

	H	S	G
21	-286.406394	76.8	-286.449632
22 MP	-157.098692	74.4	-157.140555
TS-I-o	-443.483099	105.2	-443.542317
TS-I-m	-443.475894	103.9	-443.534356
23	-443.549354	101.3	-443.606361
24	-443.543791	99.6	-443.599822
11 MCP	-155.855542	68.9	-155.894290
TS-II-o	-442.242658	100.5	-442.299237
TS-II-m	-442.239959	101.0	-442.296789
25	-442.320359	95.6	-442.374178
26	-442.316113	97.4	-442.370934
27 DCP	-233.185198	80.9	-233.230741
TS-III	-519.573695	111.6	-519.636487
28	-519.665378	105.1	-519.724532
14	-364.983812	87.5	-365.033073
TS-IV-o	-520.818052	113.0	-520.881673
TS-IV-m	-520.815860	113.7	-520.879836
29	-520.891107	103.7	-520.949457
30	-520.888625	109.9	-520.950500

Table S5. Most relevant ELF valence basins and their total populations, C–C and C–O bond formation distances and relative energies, for the structures of the IRC in which there is a relevant chemical change along the *ortho* reaction path of the *zw-type* 32CA reaction of cyclic nitrone **21** with MCP **11**. Distances are given in angstroms, Å, and relative energies with respect to **S1** are given in kcal·mol^{-1}.

Phases	*I*	*II*	*III*	*IV*	*V*	*VI*	*VII*	*VIII*	
Structures	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**25**
d1(C1-C5)	3.630	2.348	2.322	2.234	2.071	2.008	1.877	1.860	1.545
d2(O3-C4)	3.421	2.189	2.166	2.086	1.949	1.895	1.774	1.758	1.426
ΔE	0.0	16.3	16.9	17.9	14.5	11.0	0.0	-1.7	-32.0
V(C1,N2)	3.81	3.13	3.06	2.51	2.22	2.14	2.02	2.00	1.81
V(N2)		0.91	1.02	1.32	1.74	1.86	2.06	2.08	2.36
V(N2,O3)	1.47	1.36	1.35	1.31	1.23	1.20	1.14	1.13	1.00
V(C4,C5)	1.80	1.75	3.39	3.07	2.59	2.43	2.24	2.21	1.99
V'(C4,C5)	1.77	1.67							
V(C1)				0.37	0.55				
V(O3)	3.02	2.88	2.88	2.88	2.91	2.92	2.68	2.67	2.47
V'(O3)	2.92	2.98	2.97	2.94	2.87	2.84	2.74	2.71	2.50
V''(O3)							0.42		
V(C4)					0.18	0.25	0.23		
V(C5)				0.31	0.63				
V(C1,C5)						1.31	1.52	1.54	1.88
V(O3,C4)								0.72	1.32

*S6. Cartesian coordinates of the gas phase stationary points involved in the 32CA reactions of cyclic nitrone **21** with MP **22**, MCP **11** and DCP **27**, and that of cyclic dimethyl nitrone **14** with MCP **11**.*

21

C	1.39465300	-0.72306200	-0.17051900
C	1.38353400	0.79850500	0.10060900
C	-0.06411700	1.13994500	-0.03374800
C	-0.03252300	-1.16222600	0.13825000
H	2.13505900	-1.25203700	0.42945200
H	2.01338600	1.34869500	-0.60233700
H	1.75005900	1.03107100	1.10839300
H	-0.51917200	2.11728900	-0.09232000
H	-0.45521600	-1.89679600	-0.54478400
H	-0.18067300	-1.50757700	1.16383700
H	1.61927600	-0.90627800	-1.22305500
O	-2.07946900	0.01618600	-0.04859600
N	-0.83089200	0.08816800	-0.00828100

22

C	-0.00000800	-0.67737100	1.27178600
C	-0.00000800	-0.67737100	-1.27178600
C	-0.00000800	0.12507300	0.00000000
H	-0.87925900	-1.32949400	1.31727500
H	-0.00016500	-0.03748300	2.15586000
H	-0.87925900	-1.32949400	-1.31727500
H	-0.00016500	-0.03748300	-2.15586000
C	0.00001800	1.45463300	0.00000000
H	0.00001900	2.02132700	0.92549700
H	0.00001900	2.02132700	-0.92549700
H	0.87942600	-1.32924000	-1.31741500
H	0.87942600	-1.32924000	1.31741500

TS-I-o

C	0.88251500	-0.95495900	-0.40786100
N	0.68942700	0.30295000	-0.80945500
O	-0.46585700	0.66519300	-1.22171200
C	-1.69716000	-0.14633500	0.34233300
C	-0.77663100	-0.98882500	0.94402400
C	1.52892200	1.22810400	-0.03670400
C	2.74639600	0.36984600	0.29773900
C	2.19439800	-1.07784600	0.31837600
H	1.74121300	2.11204600	-0.63679500
H	0.96650100	1.53223900	0.85439100
H	3.20861200	0.65625500	1.24241200

H	2.02750400	-1.43161300	1.33948300
H	3.49826300	0.46878100	-0.48780400
H	2.87474200	-1.78512200	-0.16136800
C	-2.04732700	1.18593900	0.95348100
C	-2.71514400	-0.70774900	-0.61012100
H	-1.24956700	1.55434400	1.60238000
H	-2.95298700	1.08433400	1.56537100
H	-2.94655800	0.01318100	-1.39690000
H	-2.35136300	-1.62192200	-1.08444000
H	-0.28294100	-0.66161500	1.85611200
H	-0.89863900	-2.06294500	0.84810400
H	0.45798400	-1.74133800	-1.01542100
H	-3.64548400	-0.94465200	-0.07931200
H	-2.24221700	1.93677700	0.18606600

TS-I-m

C	0.33834800	-0.12933100	-0.99229500
N	0.91459700	0.93627900	-0.42889800
O	0.23513600	2.01308800	-0.30021800
C	-1.49907200	1.23680800	0.49931900
C	-1.44142300	-0.12619500	0.23296900
C	1.88690100	0.55452200	0.60416200
C	2.13111100	-0.94487400	0.36953300
C	1.20894500	-1.33543200	-0.81524500
H	-2.10126900	1.89162900	-0.11739400
H	2.77912500	1.17282600	0.49830800
H	1.43302100	0.77335800	1.57602200
H	1.87098400	-1.51561700	1.26152400
H	0.61803600	-2.23008200	-0.60651900
H	3.17660700	-1.15250000	0.14101700
H	1.78011400	-1.54019700	-1.72608100
H	-1.25554800	1.61507100	1.48462000
C	-2.38621300	-0.71670700	-0.79632500
C	-1.11925400	-1.06408900	1.38119100
H	-0.42631400	-0.60847500	2.09328700
H	-0.68444500	-2.01002400	1.04289900
H	-2.59068100	-0.00741600	-1.60269900
H	-1.97993800	-1.63126300	-1.24433500
H	-0.24122700	0.04017400	-1.88998500
H	-2.03314700	-1.32070600	1.92997400
H	-3.34464100	-0.98364700	-0.33645900

23

C	0.70093600	-0.97491500	-0.20436100
N	0.64478100	0.31141400	-0.91313100
O	-0.71084000	0.70933000	-0.92463000
C	-1.46866800	0.00487500	0.09884800

C	-0.43890600	-0.87473500	0.81796200
C	1.46955700	1.23340400	-0.12486400
C	2.70165000	0.37920200	0.15204400
C	2.12374300	-1.04027200	0.37386700
H	1.67742400	2.13461700	-0.70252300
H	0.97424200	1.53092400	0.81113100
H	3.27397400	0.74167700	1.00682700
H	2.09104700	-1.29751800	1.43499300
H	3.35878300	0.38552900	-0.71985500
H	2.72865700	-1.79861200	-0.12450400
C	-2.11872200	1.03988000	1.00878600
C	-2.51951200	-0.82501200	-0.63314000
H	-1.35788900	1.65289600	1.49686200
H	-2.72360100	0.55284700	1.77957700
H	-3.12075200	-0.17964500	-1.27726800
H	-2.04074700	-1.57961300	-1.26202500
H	-0.08895300	-0.39242000	1.73531500
H	-0.84917200	-1.84957900	1.08700500
H	0.50040600	-1.78078600	-0.91484500
H	-3.18298500	-1.32806600	0.07648300
H	-2.76764900	1.69864300	0.42694100

24

C	0.13188300	-0.42321100	-0.63618000
N	0.82330500	0.89736500	-0.51779300
O	-0.01317500	1.74664900	0.27386300
C	-0.87947500	0.89854600	1.00305400
C	-1.25665500	-0.19848200	0.00674800
C	2.10191100	0.67796400	0.17601200
C	2.44365600	-0.77468200	-0.13590600
C	1.07644700	-1.44486400	0.01081700
H	-1.72341300	1.50617800	1.33467300
H	2.84710700	1.39406600	-0.17389100
H	1.97481100	0.81350000	1.25872400
H	3.20088300	-1.18084300	0.53662000
H	0.85366500	-1.56474900	1.07572000
H	2.81198300	-0.86865800	-1.16183600
H	1.01119100	-2.42884300	-0.45655200
H	-0.37619900	0.47044100	1.88522900
C	-2.21990000	0.36413000	-1.04543400
C	-1.86277800	-1.43356700	0.66555500
H	-1.24462800	-1.82042700	1.47879000
H	-2.00206600	-2.23550600	-0.06527300
H	-1.80260600	1.25973300	-1.50970400
H	-2.40923700	-0.37619100	-1.82834700
H	0.01573400	-0.65121300	-1.69986200
H	-2.84557300	-1.19379200	1.08173800
H	-3.17993000	0.62654800	-0.59037100

11

C	0.76828500	-0.93024100	0.00000000
C	-0.76806200	-0.93039300	0.00000000
C	0.00000000	0.31730800	0.00000000
H	1.27192900	-1.23066200	0.91327500
H	1.27192900	-1.23066200	-0.91327500
H	-1.27163300	-1.23090700	0.91328300
H	-1.27163300	-1.23090700	-0.91328300
C	-0.00021700	1.63257100	0.00000000
H	0.92823300	2.19400200	0.00000000
H	-0.92886100	2.19367000	0.00000000

TS-II-o

C	-1.01009400	0.76499500	-0.71280900
N	-0.67384300	-0.52058200	-0.67596300
O	0.50494100	-0.88683300	-1.00267400
C	1.61315500	0.38118400	0.21683400
C	0.73305300	1.38044900	0.52659100
C	-1.38032200	-1.21245200	0.41068000
C	-2.67852700	-0.41702300	0.52687900
C	-2.30563400	0.99591500	0.01068900
H	-1.50641100	-2.26256900	0.15069600
H	-0.74899400	-1.13997400	1.30515100
H	-3.06419500	-0.40197100	1.54602200
H	-2.15514600	1.70110500	0.83244000
H	-3.44422100	-0.85687700	-0.11518600
H	-3.07808000	1.41593700	-0.63784800
C	2.48930200	-0.61750800	0.85654000
C	2.93571100	0.16904300	-0.38254400
H	2.27377100	-1.66932000	0.71509000
H	2.94035900	-0.35835100	1.81000300
H	2.98618800	-0.37847700	-1.31667200
H	3.68843700	0.94034900	-0.25322900
H	0.22985600	1.37124300	1.48984800
H	0.82672000	2.34916300	0.04745200
H	-0.65076800	1.36085900	-1.53779900

TS-II-m

C	0.42226300	-0.13649300	-0.98193900
N	1.03030200	0.86297000	-0.34701400
O	0.51591500	2.02649600	-0.33322800
C	-1.47573100	1.48440600	0.27112400
C	-1.45348500	0.12800900	0.09143400
C	1.75440000	0.36468900	0.83090200
C	2.08688100	-1.08191800	0.45789500

C	1.08620000	-1.44279700	-0.67296400
H	-1.89204200	2.14099300	-0.48208500
H	2.61993400	0.99871200	1.01861100
H	1.06634800	0.44174900	1.68126700
H	1.99569400	-1.74903800	1.31497400
H	0.35298000	-2.18953500	-0.35689400
H	3.11121300	-1.15504000	0.08926900
H	1.59216300	-1.85525300	-1.54978000
H	-1.29843900	1.91844600	1.24694000
C	-2.34052500	-0.91867800	-0.45998300
C	-1.75138600	-1.04026000	0.94898200
H	-2.42327000	-0.89807800	1.78964100
H	-1.00685100	-1.81485000	1.11150800
H	-3.40188300	-0.71180600	-0.54916600
H	-1.95834900	-1.60453000	-1.21294800
H	-0.06862700	0.08372200	-1.91911600

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C	-0.79222700	0.95830100	-0.57627800
N	-0.69111100	-0.48163900	-0.97547400
O	0.69672400	-0.81646100	-0.98364200
C	1.33269500	0.07750800	-0.10701800
C	0.65591900	1.40574800	-0.33189700
C	-1.40785500	-1.28064100	0.03143600
C	-2.48977600	-0.33199000	0.53224800
C	-1.71573900	0.98334400	0.64978700
H	-1.79527000	-2.19283500	-0.42498900
H	-0.74039100	-1.55690700	0.85653200
H	-2.93086400	-0.66058500	1.47459800
H	-1.11790600	0.97408700	1.56756300
H	-3.29100200	-0.24275800	-0.20723800
H	-2.35402500	1.86829500	0.67296100
C	1.78753100	-0.40413300	1.24703600
C	2.78020100	-0.13407300	0.12846800
H	1.60628500	-1.44294100	1.49279800
H	1.75426600	0.28516200	2.08351800
H	3.22879200	-0.99634000	-0.34941800
H	3.41867600	0.73874300	0.19897000
H	0.74625400	2.08731800	0.51547300
H	1.07284900	1.88703000	-1.21988400
H	-1.23817300	1.51051000	-1.40611800

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C	0.18097500	-0.18797700	-0.93949400
N	1.00756100	0.93675200	-0.49511400
O	0.09608100	1.98674400	-0.24056000
C	-1.13246100	1.42696200	0.25207200

C	-1.07363300	-0.05923000	-0.07224000
C	1.65689500	0.47986800	0.74864100
C	1.95388200	-1.00792700	0.49967200
C	1.07831700	-1.39591600	-0.71894800
H	-1.94246200	1.94384200	-0.26889900
H	2.54996500	1.07737000	0.93290600
H	0.98290900	0.60155800	1.60597900
H	1.70234700	-1.60015000	1.38105200
H	0.50960000	-2.31432800	-0.56130200
H	3.00956600	-1.17737000	0.28410600
H	1.69845400	-1.54954800	-1.60354700
H	-1.23172800	1.60499400	1.32937900
C	-2.30224600	-0.88268200	-0.29320800
C	-1.47870800	-1.07893400	0.95545900
H	-1.88296500	-0.70666800	1.89063700
H	-0.90464400	-1.99353800	1.05001500
H	-3.26937500	-0.40157000	-0.19873500
H	-2.25661900	-1.65657300	-1.05256100
H	-0.08474300	-0.04421900	-1.99047000

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C	-1.89944700	-0.76843800	0.00024100
C	-1.90056200	0.76787900	-0.00000800
C	-0.65143600	0.00062300	-0.00018500
H	-2.19885200	-1.27183300	0.91416400
H	-2.20015300	-1.27277300	-0.91267700
H	-2.20156900	1.27178200	0.91305200
H	-2.20113100	1.27087600	-0.91376600
C	0.65156700	0.00100200	-0.00119100
C	1.90011000	0.76799400	0.00049800
C	1.89961100	-0.76850600	0.00016000
H	2.20283300	1.27122200	-0.91250000
H	2.20016400	1.27175100	0.91400200
H	2.20107100	-1.27169900	-0.91314800
H	2.19858300	-1.27265000	0.91378400

TS-III

C	-1.05638900	0.09526300	-1.00063500
N	-0.87976500	-1.09315200	-0.44634400
O	0.22309800	-1.71485200	-0.57207100
C	1.56345300	-0.17885800	0.02681800
C	0.78517000	0.92829600	0.01645600
C	-1.65959300	-1.21481600	0.79459600
C	-2.82730300	-0.25457900	0.56468000
C	-2.30982800	0.74237700	-0.50527500
H	-1.94448600	-2.25559400	0.94277300
H	-0.99932600	-0.90301400	1.61187100

H	-3.12991900	0.24557500	1.48437400
H	-2.09097400	1.72685700	-0.08122900
H	-3.69262900	-0.79720600	0.18003200
H	-3.03544100	0.90079200	-1.30706600
C	2.42720300	-0.97796700	0.91013100
C	2.78813900	-0.73073100	-0.56126100
H	2.11984100	-1.98133400	1.17785100
H	2.99810500	-0.44927600	1.66916400
H	2.69429100	-1.57319800	-1.23689400
H	3.60324000	-0.04692700	-0.78047200
H	-0.58252200	0.29824000	-1.94929200
C	0.85174100	2.32616600	-0.45214400
C	0.43544600	1.98725400	0.98414200
H	1.82582300	2.78213400	-0.60271800
H	0.07768100	2.71272800	-1.11231000
H	1.14206700	2.20649900	1.77983700
H	-0.60041700	2.17017300	1.26000300

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C	-0.70007700	0.90040300	-0.47953100
N	-1.09795000	-0.43888300	-1.01468200
O	0.08004700	-1.24677700	-1.05212400
C	0.94670200	-0.73506100	-0.07202000
C	0.77850600	0.75027900	-0.15136300
C	-2.09127000	-1.01534000	-0.09522100
C	-2.80396000	0.21053000	0.46108000
C	-1.63122700	1.16244800	0.71328400
H	-2.74435200	-1.70075900	-0.63757700
H	-1.60127800	-1.56487400	0.71758900
H	-3.38010900	-0.01258500	1.36037100
H	-1.12404600	0.88717700	1.64334000
H	-3.48509700	0.62679200	-0.28684000
H	-1.92734200	2.21009300	0.78922300
C	1.12971500	-1.48409300	1.22320000
C	2.21671500	-1.45855400	0.16267200
H	0.58726900	-2.41361500	1.34172700
H	1.28710000	-0.91358400	2.13167100
H	2.37456000	-2.36362400	-0.41055700
H	3.11067100	-0.87372200	0.35216000
H	-0.84863700	1.64483500	-1.26593100
C	1.54468000	1.72224400	0.68512000
C	1.81990000	1.61693400	-0.79585000
H	2.28968800	1.32855500	1.36917600
H	1.02483100	2.60080500	1.05007800
H	2.74499500	1.14760300	-1.10931800
H	1.47892100	2.42455500	-1.43357200

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C	0.71784600	-1.38028600	0.00026800
C	1.97194400	-0.47239300	0.00004700
C	1.40811400	0.90524900	0.00004900
C	-0.50679200	-0.44466400	0.00003500
H	0.70454800	-2.02673300	0.87883100
H	2.60287300	-0.64574300	-0.87743700
H	2.60324700	-0.64570900	0.87726400
H	1.94971600	1.83993600	0.00004700
H	0.70456100	-2.02733000	-0.87785200
O	-0.64571200	1.93649400	-0.00002500
N	0.11128300	0.93535600	0.00003500
C	-1.35929500	-0.55604000	1.25819700
H	-2.11283500	0.23226600	1.26646700
H	-1.85541400	-1.52939100	1.28387400
H	-0.74127200	-0.45659500	2.15459700
C	-1.35871500	-0.55617800	-1.25852600
H	-0.74029200	-0.45646700	-2.15462100
H	-1.85451000	-1.52968600	-1.28452200
H	-2.11250900	0.23188100	-1.26710400

TS-IV-o

C	-0.44393900	1.36429700	-0.63131800
N	-0.45892600	0.04054800	-0.75365900
O	0.60547700	-0.57840400	-1.09800700
C	1.99283500	0.28062600	0.15843000
C	1.38095000	1.42743400	0.59261800
C	-1.48376400	-0.61143700	0.11469200
C	-2.50224200	0.53187100	0.24401500
C	-1.68050300	1.83013600	0.08500600
H	-3.04127500	0.48582700	1.19141300
H	-1.41273800	2.26083900	1.05408500
H	-3.23550700	0.46124500	-0.56325400
H	-2.22376100	2.59709600	-0.47061800
C	2.66206700	-0.93148200	0.66362200
C	3.21918100	-0.14336100	-0.52785100
H	2.23080700	-1.90078900	0.44378700
H	3.18777100	-0.86319200	1.61135600
H	3.11555300	-0.60373700	-1.50400600
H	4.12181200	0.44144500	-0.38117700
H	0.92534800	1.45745800	1.57747900
H	1.71056700	2.38348800	0.19987100
H	0.07307800	1.93829000	-1.38488700
C	-0.87000400	-1.00474000	1.45881800
H	-1.60993000	-1.54812800	2.05177300
H	-0.00338100	-1.64848600	1.30423900
H	-0.54969300	-0.13092100	2.02939000
C	-2.01957900	-1.83651000	-0.61174600
H	-2.80674200	-2.31247300	-0.02123200

H	-2.42947100	-1.55965100	-1.58600200
H	-1.21378400	-2.55592300	-0.77027700

TS-IV-m

C	0.24646300	0.53673200	-1.05788600
N	-0.65922700	-0.39615000	-0.77129200
O	-0.37650400	-1.62900900	-0.92731900
C	1.53145200	-1.69328000	-0.00864700
C	1.85802700	-0.36225300	0.05966000
C	-1.63129400	0.04419100	0.27387600
C	-1.58574900	1.56938900	0.08197000
C	-0.21099300	1.87458700	-0.55694800
H	1.89464900	-2.31305800	-0.81815700
H	-1.73547800	2.09482900	1.02617200
H	0.49719000	2.27712200	0.17274300
H	-2.38251700	1.87664800	-0.59946200
H	-0.28730900	2.61002700	-1.36072300
H	1.13712600	-2.21142600	0.85626700
C	3.04915900	0.46016900	-0.24695400
C	2.37080100	0.52877200	1.12363600
H	2.88432700	0.07741300	1.96681800
H	1.85424000	1.45227300	1.37267600
H	4.01941800	-0.02131800	-0.31262000
H	2.94310000	1.33395400	-0.88628500
H	0.84452900	0.40626500	-1.94832500
C	-1.14034800	-0.39503200	1.65325900
H	-1.87397600	-0.10814200	2.41067700
H	-1.02233000	-1.47995900	1.67843300
H	-0.18154300	0.06342500	1.90241400
C	-2.98686700	-0.57369300	-0.03818400
H	-3.72899200	-0.24658700	0.69477500
H	-3.32549200	-0.28128300	-1.03508600
H	-2.91422600	-1.66255200	-0.00541100

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C	-0.15721000	1.44539500	-0.51882600
N	-0.47520400	0.04915600	-0.90352400
O	0.74135300	-0.67507300	-0.96108200
C	1.69848300	-0.02006400	-0.15325700
C	1.32939800	1.44862700	-0.11996800
C	-1.48634400	-0.52316700	0.02180400
C	-2.27149100	0.74732400	0.38231900
C	-1.18078700	1.80525000	0.56647200
H	-2.89088400	0.60440000	1.27001400
H	-0.73100100	1.71935500	1.55998400
H	-2.92904300	1.02140000	-0.44838600
H	-1.55421500	2.82535800	0.46282200

C	2.31143500	-0.74494700	1.01115300
C	3.09327800	-0.52020900	-0.27059400
H	1.97682000	-1.75599800	1.20414200
H	2.58261100	-0.17276300	1.89205500
H	3.24596900	-1.38326000	-0.90745800
H	3.89896600	0.20520700	-0.27463200
H	1.49099700	1.88917200	0.86588700
H	1.92444700	2.00690100	-0.84604200
H	-0.30224900	2.07843100	-1.39792500
C	-0.91329300	-1.18529700	1.27994700
H	-0.28786300	-2.03578000	1.00699500
H	-0.31037100	-0.49979900	1.87848300
H	-1.73540400	-1.55141200	1.90092000
C	-2.32369000	-1.53849000	-0.75082400
H	-3.14471900	-1.91964600	-0.13568700
H	-2.73604000	-1.07818800	-1.65088200
H	-1.70108900	-2.38341500	-1.05632700

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C	0.49393200	0.51366100	-0.99388800
N	-0.63974300	-0.40212200	-0.91043000
O	-0.08838600	-1.69443100	-0.75094400
C	1.20585300	-1.60422400	-0.13739800
C	1.55129700	-0.12624900	-0.09324000
C	-1.54206800	0.02474100	0.21715600
C	-1.07859400	1.46552900	0.54631100
C	-0.09370200	1.84797200	-0.56650900
H	1.89685500	-2.17254000	-0.76719100
H	-0.57719600	1.47857300	1.51677600
H	0.66729300	2.56103300	-0.24132800
H	-1.92083500	2.15783700	0.60512200
H	-0.61828200	2.29408800	-1.41475100
H	1.18043100	-2.05403800	0.86175300
C	2.96802800	0.35160700	-0.04265100
C	2.07698700	0.50931300	1.16383800
H	2.25545600	-0.13921200	2.01478700
H	1.75293100	1.51019600	1.42467800
H	3.76008600	-0.38807800	-0.00439600
H	3.21469200	1.24722300	-0.60355200
H	0.86633500	0.53316400	-2.02312900
C	-1.45187400	-0.88161600	1.44399300
H	-1.68490800	-1.91529900	1.18456200
H	-0.45711200	-0.85017700	1.89437700
H	-2.16866100	-0.53887000	2.19524100
C	-2.96680300	0.00711600	-0.33904800
H	-3.68880000	0.33157800	0.41711900
H	-3.04246600	0.66982200	-1.20475600
H	-3.22886400	-1.00209300	-0.66613000