Electronic Supporting Information

Why is Phenyl Azide so Unreactive in [3+2] Cycloaddition Reactions? Demystifying Sustmann's Paradigmatic Parabola

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1. ELF analysis of the electronic structure of the reagents

The topological analysis of the Electron Localization Function[1] (ELF) permits a quantitative characterization of the electron density distribution in a molecule,[2] establishing a correlation between its electronic structure and its reactivity. Consequently, an ELF topological analysis of the electronic structure of the simplest azide **9**, phenyl azide, **6**, two substituted phenyl azides, **42** and **43**, and three selected ethylene derivatives, **22**, **30**, and **40**, was performed. ELF valence basins, basin attractor positions, and the most relevant valence basin populations, are shown in Figures S1 and S2.

ELF of the simplest azide **9** shows the presence of two disynaptic basins, V(N1,N2) and V'(N1,N2), integrating a total of 4.13 e, one V(N2,N3) disynaptic basin integrating 2.43 e, and two monosynaptic basins, V(N1) and V(N3) integrating 3.79 and 3.46 e, respectively. While the population of the two V(N1,N2) and V'(N1,N2) disynaptic basins allows relating the N1–N2 bonding region to a double bond, that of the V(N2,N3) disynaptic basin allows associating the N2–N3 bonding region with a populated single bond within Lewis's bonding model. The V(N1) and V(N3) monosynaptic basins may be associated with non-bonding electron density regions at the N1 and N3 nitrogens. The absence of any *pseudoradical* or carbenoid carbon at this inorganic species allows classifying it as a zwitterionic three-atom component (TAC).[3]

Substitution of the hydrogen of simplest azide **9** by the phenyl group practically does not modify the ELF of phenyl azide **6** (see Figure S1). The valence basin population changes are less than 0.08 e (V(N3)). The total ELF valence basin population of the -NNN core of phenyl azide **6**, 13.78 e, has decreased by only 0.03 e with respect to that of simplest azide **9**, indicating that the presence of the phenyl substituent does not cause any remarkable change in the ground state (GS) electronic structure of the azide TAC core.

Interestingly, the presence of a strong electron-withdrawing (EW) $–NO_2$ nitro group in *p*-nitro-phenyl azide **42** or a strong electron-releasing (ER) $–OCH_3$ methoxy group in *p*-methoxy-phenyl azide **43** neither cause any remarkable change in the GS electronic structure of the TAC core of phenyl azide **6** (see Figure S1). While the total ELF valence basin population of the -NNN core of *p*-nitro-phenyl **42** has decreased by only 0.05e with respect to that of phenyl azide **6**, that of *p*-methoxy-phenyl azide **43** has increased by only 0.01 e. Consequently, ELF of the four azides indicates that substituting the hydrogen of the simplest azide **8** by aryl substituents does not modify the GS electronic structure of these zwitterionic TACs.

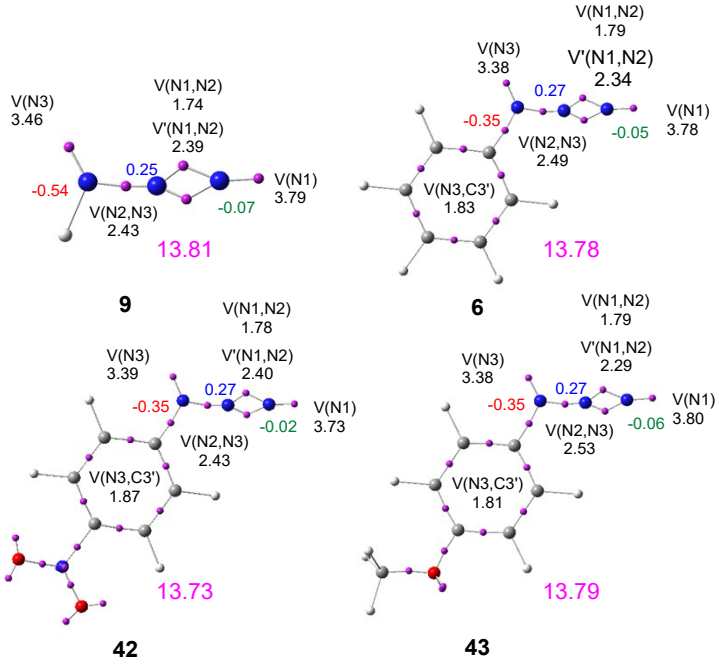


Figure S1. ELF basin attractor positions, together with the most relevant valence basin populations and natural atomic charges of azides **6**, **9**, **42** and **43**, computed at the *ω*B97x-D/6-311G(d,p) level in gas phase. Valence basin populations and natural atomic charges are given in an average number of electrons, e. Negative charges are colored in red, positive in blue, and negligible in green.

ELF of strained cyclopentene **30** shows the presence of two disynaptic basins, V(C4,C5) and V(C4,C5), integrating a total of 3.50 e. This behavior allows relating the C4–C5 bonding region of cyclopentene **30** to an underpopulated C4–C5 double bond according to Lewis's bonding model. The presence of a strong ER amino group in vinyl amine **22** increases the electron density of the C4–C5 bonding region by only 0.06 e, while the presence of an EW nitrile group in acrylonitrile **40** decreases this electron density by 0.17 e because of a stronger polarization of the C4–C5 bonding region of these substituted ethylenes.

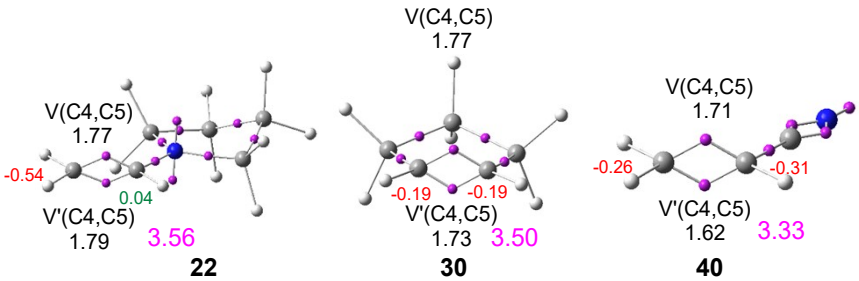


Figure S2. ELF basin attractor positions, most relevant valence basin populations and natural atomic charges of ethylenes **22**, **30** and **40**, at the *ω*B97x-D/6-311G(d,p) level in gas phase. Valence basin populations and natural atomic charges are given in an average number of electrons, e. Negative charges are colored in red and negligible charges are colored in green.

Finally, the natural atomic charges of the four azides and the three ethylenes, obtained by a Natural Population Analysis[4,5] (NPA), were studied (see Figures S1 and S2). While the two N1 and N3 nitrogens of simplest azide **9** are negatively charged by –0.07 and –0.53 e, respectively, the central N2 nitrogen is positively charged by +0.25. Note that the negative charge of the N3 nitrogen is mainly a consequence of the higher electronegative character of the nitrogen with respect to the attached hydrogen, which is positively charged by +0.36 e. This charge distribution, which does not correspond with that in the traditional 1,2-dipolar structure of azides, is a consequence of the total electron density distribution around the NNN core of this TAC, which is only determined by the presence of the three nitrogen nuclei and not by any resonance analysis.[3]

The substitution of the hydrogen atom in the simplest azide **6** by the phenyl group only decreases the negative charge of the N3 nitrogen by 0.19 e due to the delocalization of the electron density of the N3 nitrogen in the aromatic ring, in agreement with the reduction of the population of the V(N3) monosynaptic basin of phenyl azide **6**. Interestingly, substitution on the aromatic ring of phenyl azide **6** by an EW group in **42** or an ER group in **43** does not cause any remarkable change in the charge distribution with respect to that in phenyl azide **6**, supporting the previous finding that these substitutions do not modify the GS electronic structures of the azide core of these TACs.

NPA of the three ethylenes shows that charges depend on the substitution of the C4–C5 double bond of the ethylene. Due to the symmetry of cyclopentene **30**, the two carbons are negatively charged by –0.19 e. These negative charges result from the more electronegative character of the carbon than the hydrogen attached to them.

The presence of the ER amine group in the vinyl amine **22** strongly polarizes the electron density of the C4–C5 double bond towards the terminal C4 carbon, which is negatively charged by –0.54 e. The presence of the EW nitrile group in acrylonitrile **40** causes a minor effect; although the substituted C5 carbon gathers a higher negative charge, both C4 and C5 carbons are more negatively charged than those in cyclopentene **30**. The increase of the negative charge at these carbons, 0.19 e, can be related to the depopulation of the two V(C4,C5) and V(C4,C5) disynaptic basins, 0.17 e, in acrylonitrile **40** (see Figure S2).

2. Analysis of the reactivity indices at the GS of the reagents

The reactivity indices[6,7] defined within DFT are powerful tools for understanding the reactivity in polar cycloaddition reactions.[8] The reactivity indices were calculated at the B3LYP/6-31G(d) computational level since it was used to establish the electrophilicity and nucleophilicity scales.[7] The global reactivity indices, namely, the electronic chemical potential μ, chemical hardness η, electrophilicity ω, and nucleophilicity *N*, for the azides are gathered in Table S1. At the same time, those at the substituted ethylenes are given in Table S2.

The simplest azide **9** presents a very low electrophilicity ω index,[9] ω = 0.66 eV, and nucleophilicity *N* index,[10] *N* = 1.81 eV, values, being classified as a marginal electrophile and a marginal nucleophile within the electrophilicity and nucleophilicity scales.[7] Consequently, due to the zwitterionic nature of this inorganic species, these reactivity indices show that the simplest azide **9** will be one of the least reactive TACs. In addition, the high chemical hardness η of simplest azide **9**, η = 8.09 eV, indicates the very low tendency of this species to exchange electron density. This behavior can be understood because of the three electronegative nitrogen atoms in the core of azide TACs.

Phenyl azide **6** presents an electrophilicity ω index of 1.27 eV and nucleophilicity *N* index of 2.92 eV, being classified as a moderate electrophile and on the borderline between moderate and strong nucleophiles. The presence of the phenyl substituent in the azide core should substantially modify its reactivity with respect to that of the simplest azide **9**, despite the low effect of substitution on the electronic structure of the TAC. It should be emphasized that phenyl azide **6** is not "ambiphilic", as has been suggested,[11] since it has neither a strong electrophilic and a strong nucleophilic character (see Section S3 in ESI).[12]

As expected, the presence of a strong EW $–NO_2$ group in the phenyl substituent of **42** and a strong ER $–OCH_3$ group in the phenyl substituent of **43** modify their electrophilicity ω index, 2.66 eV, and nucleophilicity *N* index, 3.47 eV, respectively, of these substituted azides, which are classified either as strong electrophiles or strong nucleophiles. Consequently, they are expected to participate in polar *zw-type* 32CA reactions with low activation energies. However, it is found that the corresponding electronic activation does not substantially modify the experimental reactivity of phenyl azide **6**.[13]

Table S1. B3LYP/6-31G(d) global electronic chemical potential μ, chemical hardness η, electrophilicity ω, and nucleophilicity *N*, in eV, of selected azides and nitrone **14**.

	μ	η	ω	*N*
42	-4.82	4.37	2.66	2.12
6	-3.62	5.17	1.27	2.92
44	-3.85	6.19	1.20	2.17
43	-3.27	4.76	1.12	3.47
14	-2.97	5.17	0.85	3.57
9	-3.26	8.09	0.66	1.81

Table S2 presents the reactivity indices of the 25 ethylenes selected in this MEDT study, ordered from largest to smallest nucleophilicity *N* index. Ethylenes **18** - **28** have nucleophilicity *N* indices higher than 3.0 eV, thus being classified as strong nucleophiles participating in polar reactions. The very high nucleophilicity *N* index of ethylenes **18** - **23**, higher than 4.0 eV, allows categorizing them as supernucleophiles participating towards strong electrophiles in highly polar reactions.[8] Note that TACs **18** - **24** are vinyl amines. Compounds **29** - **33** have nucleophilicity *N* indices between 2.00 and 2.84 eV, being classified as moderate nucleophiles. These ethylenes will react only in polar reactions with very strong electrophilic species. Note that some of them are strained cyclic ethylenes. Finally, ethylenes **5**, **15**, **34** - **41** have nucleophilicity *N* indices lower than 2.0 eV, being classified as marginal nucleophiles. These species will never participate in a polar reaction as nucleophiles. However, ethylenes **15**, **36** - **41** have electrophilicity ω indices higher than 1.50 eV, being classified as strong electrophilic species.

The electronic chemical potential[14] μ of simplest azide **9** is –3.26 eV. The presence of the phenyl group in phenyl azide **6** slightly decreases its electronic chemical potential μ to –3.62 eV. The electronic chemical potentials μ of the supernucleophiles **18** - **23**, between –1.42 and –1.87 eV, are higher than that of phenyl azide **6**. Consequently, along the corresponding polar 32CA reactions, the flux of the electron density will take place from ethylenes **18** – **23** towards phenyl azide **6**, the 32CA reactions being classified as reverse electron density flux (REDF).[15,16] On the other hand, strong electrophilic ethylenes **15**, **36** - **41** have electronic chemical potentials μ lower than –4.11 eV; consequently, it is expected that along a polar reaction, the flux of the electron density will take place from phenyl azide **6** towards these electrophilically activated ethylenes, and now the 32CA reactions are classified as forward electron density flux (FEDF).[15,16] Note that Sustmann classified all

these 32CA reactions indistinctly as "of type II, in which the HOMO and LUMO energies of the reagents should be considered".[17]

Table S2. B3LYP/6-31G(d) global electronic chemical potential μ, chemical hardness η, electrophilicity ω, and nucleophilicity *N*, in eV, of ethylenes **5**, **15**, **18 - 41.**

	μ	η	ω	*N*
18	-1.42	6.27	0.16	4.57
19	-1.53	6.22	0.19	4.49
20	-1.38	6.65	0.14	4.41
21	-1.54	6.36	0.19	4.40
22	-1.88	6.38	0.28	4.05
23	-1.87	6.51	0.27	4.00
24	-1.94	7.30	0.26	3.53
25	-2.36	6.97	0.40	3.27
26	-2.37	6.97	0.40	3.27
27	-2.45	6.99	0.43	3.18
28	-3.43	5.20	1.13	3.09
29	-2.79	6.98	0.56	2.84
30	-3.53	5.51	1.13	2.83
31	-2.72	7.24	0.51	2.78
32	-2.71	7.28	0.50	2.77
33	-2.79	7.19	0.54	2.74
34	-4.11	6.22	1.36	1.90
35	-4.11	6.24	1.35	1.89
36	-4.58	5.61	1.87	1.73
37	-4.32	6.17	1.51	1.72
38	-4.87	5.23	2.26	1.64
39	-4.42	6.43	1.52	1.48
40	-4.70	6.34	1.74	1.25
41	-4.70	6.35	1.74	1.24
15	-5.33	5.45	2.61	1.07
5	-3.37	7.77	0.73	1.87

Along a polar cycloaddition reaction involving non-symmetric species, the most favorable reaction path involves the two-center interaction between the most electrophilic and the most nucleophilic centers of the reagents.[18] Many studies have shown that the analysis of the electrophilic P_k^+ and nucleophilic P_k^- Parr functions[19] resulting from the excess of spin electron density gathered via the global electron density transfer (GEDT),[20] is one of the most accurate and insightful tools for the study of the local reactivity in polar and

ionic processes. Hence, the electrophilic P_k^+ and nucleophilic P_k^- Parr functions of azides **6**, **9**, and **44**, and those of nucleophilic ethylene **18** and electrophilic ethylene **40** are analyzed (see Figures S3).

Analysis of the electrophilic and nucleophilic Parr functions of phenyl azide **6** shows that they are mainly concentrated in the aromatic ring. Consequently, the regioselectivity of 32CA reactions aryl azides cannot be explained using these local indices. However, a different behavior is found when analyzing the Parr functions of aliphatic azides **9** and **44**. The two azides present a similar local reactivity in which the N1 nitrogen, 0.56 (**44**), is the most electrophilic center; thus, this center is the preferred one for a nucleophilic attack, in complete agreement with the experimental *meta* regioselectivity experimentally observed

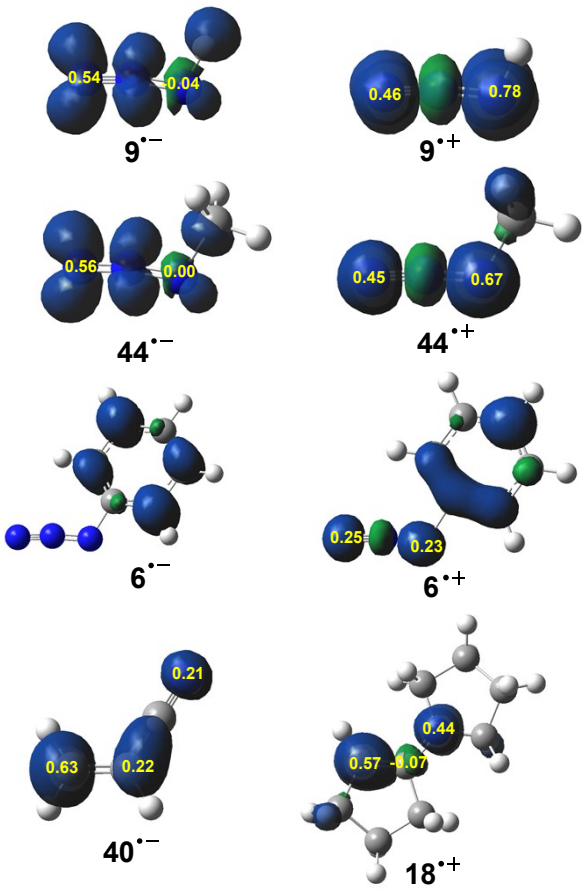


Figure S3. 3D representations of the Mulliken atomic spin densities of the radical anion and the radical cation of azides **9, 44**, and **6,** as well as the radical anion of electrophilic acrylonitrile **40**, and the radical cation of nucleophilic vinyl amine **18**, including the values of the electrophilic P_k^+ and nucleophilic P_k^- Parr functions. While blue areas indicate local electrophilic or nucleophilic activation, green areas indicate local deactivation.

towards nucleophilic ethylenes. On the other hand, the N3 nitrogen, 0.67 (**44**), is the most nucleophilic center of these species, followed by the N1 nitrogen, 0.45 (**44**). Consequently, a mixture of the two regioisomers, in which the *ortho* regioisomer will be the major one, will be expected in the polar *zw-type* 32CA reactions towards electrophilic ethylenes.

The C4 carbon of vinyl amine **18** is the most nucleophilic center, $P_k^- = 0.57$, of this ethylene, followed by the amine N6 nitrogen, $P_k^- = 0.44$. Note that the C5 carbon is nucleophilically deactivated. On the other hand, the C4 carbon of acrylonitrile **40**, $P_k^+ = 0.63$, is three times more electrophilically activated than the C5 carbon, $P_k^+ = 0.22$. Consequently, it is expected that along the nucleophilic attacks to azides in REDF reactions, the most favorable reaction path will be that initialized by the two-center interactions between the C4 carbon of the ethylene and the N1 nitrogen of azides, i.e., the *meta* reaction path (see later), while along the electrophilic attacks to azides in FEDF reactions, the most favorable reaction path will be that initialized by the two-center interactions between the C4 carbon of the ethylene and the N3 nitrogen of azides, i.e. the *ortho* reaction path.

3.The chemical meaning of the "ambiphilic species" concept

In 1995, Kondo et al.[21] reported that (η^3-allyl)ruthenium(II) complexes could function as both nucleophile and electrophile, i.e., as an ambiphile, as they smoothly react with both aldehydes and $NaCH(COOMe)_2$ under extremely mild reaction conditions to give the corresponding allylated products in good to high yields.[21] More recently, in 2009 Ayers et al.[22] indicated that ambiphilic reagents act as either electrophiles or nucleophiles, depending on the reaction partner. Some ambiphilic reagents even accept (electrophilic behavior) and donate (nucleophilic behavior) electrons at the same time.[22] It is therefore important to emphasize that a species that reacts with either nucleophiles and electrophiles is not necessarily ambiphilic (note that cyclopentadiene, which is not ambiphilic, is able to react with both electrophilic and nucleophilic reagents). Instead, an ambiphilic species is both a strong nucleophile and a strong electrophile, participating in polar reactions toward strong electrophiles and strong nucleophiles under mild conditions.

TACs are species with a chemical framework of three heavy nuclei embedded in the electron density corresponding to about eight electrons. This structure makes many TACs behave as a strong nucleophilic character, $N > 3.00$, and others behave as a low electrophilic character, $\omega < 1.00$.[3] As a result, TACs as nitrones generally behave as good nucleophiles toward electrophilic ethylenes in polar 32CA reactions.[23] Note that nitrone **14** has a nucleophilicity *N* index of 3.57 eV, being classified as a strong nucleophile.

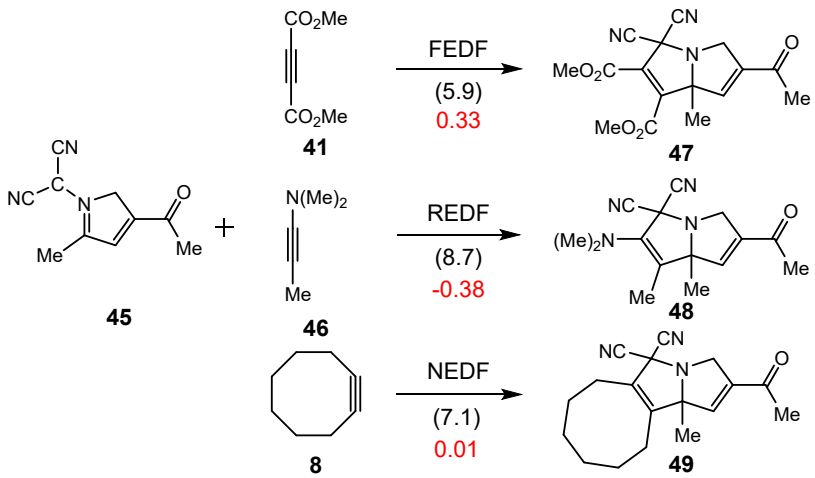
The simplest azomethine ylide (AY) **1**, a *pseudodiradical* species, is one of the most reactive TACs participating in *pdr-type* 32CA reactions (see Scheme 1 in the Manuscript).[3] AY **1** is a supernucleophile,[3] $N = 5.07$ eV, and a marginal electrophile, $\omega = 0.37$ eV. Consequently, this AY **1** participates in polar *pdr-type* 32CA reactions even with poor electrophilic ethylenes. However, the structure and reactivity of the simplest TACs can be modified with the substitution.

The 32CA reactions of cyclic AY **45** with a series of acetylenes, experimentally reported by Sauer,[24] were recently studied within MEDT (Scheme S1).[12] Analysis of the reactivity indices of cyclic AY **45** allowed characterising this TAC as a strong electrophile, $\omega = 3.92$ eV, and a strong nucleophile, $N = 3.34$ eV, thus participating in polar 32CA reactions towards both electrophilic and nucleophilic acetylenes such as dimethyl acetylene dicarboxylate **41**, a strong electrophile, and *N*,*N*-dimethylpropynamine **44**, a strong nucleophile. Again, the loss of the ring strain present in cyclooctyne **8** along an SP-32CA reaction of cyclic AY **45** explains its participation in a non-polar 32CA reaction of NEDF

with a low activation energy comparable to polar reactions (see the GEDT of the three 32CA reactions in Scheme S1).[12] This MEDT study, which allowed explaining the experimental kinetic data reported by Sauer,[24] classifying cyclic AY **45** as an "amphiphilic species" able to react quickly with both electrophilic and nucleophilic ethylenes in a polar process due to its strong electrophilic and nucleophilic character, against the simplest AY **1** which only reacts with electrophilic ethylenes in polar processes. Although cyclic AY **45** reacted easily with cyclooctyne **8** along an SP-32CA reaction, in this case the behaviour of AY **45** cannot be classified as amphiphilic as the reaction was non-polar; the GEDT was 0.001e.

Consequently, the analysis of the reactivity indices of phenyl azide **6**, which classifies this TAC as moderate electrophile and moderate nucleophile, does not characterize phenyl azide **6** as an ambiphilic species, as suggested.[11] Note that the GEDT at **TS-42o** of the 32CA reaction of phenyl azide **6** with acrylonitrile **40**, a strong electrophile, is only of 0.04 e (see Table 4 in the Manuscript). This value indicates the non-polar character of the 32CA reaction, which agree with the high activation energy associated with this *zw-type* 32CA reaction; 17.2 kcal·mol^{-1} (see Table 3 in the Manuscript).

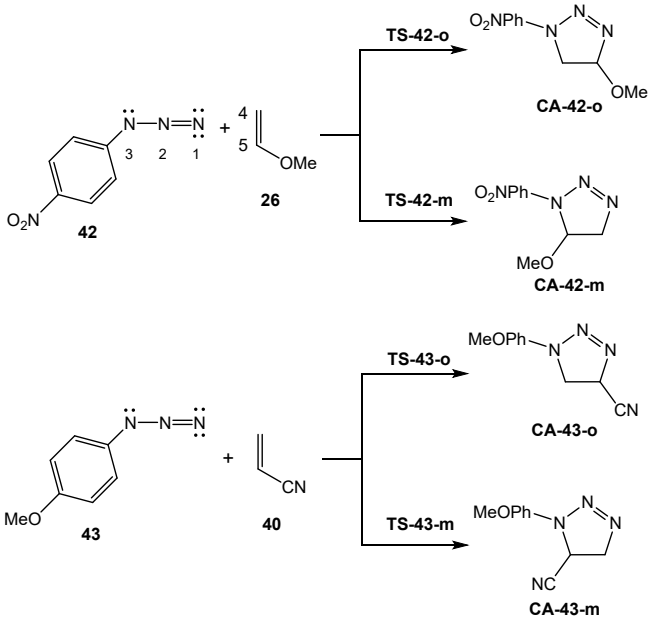
It is worth emphasizing that in 2006, Houk reported a review entitled "*Conceptual, qualitative, and quantitative theories of 1,3-dipolar and Diels–Alder cycloadditions used in synthesis,*" in which "the application of conceptual density functional theory (DFT) for predicting reactivity and regioselectivity" in this type of organic reactions was highlighted.[25]



Scheme S1. 32CA reactions of cyclic AY **42** with electrophilic acetylene **41**, nucleophilic acetylene **46**, and strained cyclooctyne **8**. The MPWB1K/6-311G(d,p) relative energies with respect to reagents are given in kcal·mol^{-1}. In parenthesis, the GEDT at the TSs in red are given in average of electrons

4. Study the origin of the low electronic activation of the zw-type 32CA reactions of the substituted phenyl azides

The 32CA reactions of aryl azides of different electronic nature with nucleophilic and electrophilic ethylenes have shown that substitution on the aromatic ring does not substantially modify the reactivity of phenyl azide **6**,[13] unlike other similar zwitterionic TACs such as *C*,*N*-diaryl nitrones.[23]To understand this behavior of aryl azides, the 32CA reaction of *p*-nitro-phenyl azide **42**, a strongly electrophilic azide, with nucleophilic enol ether **26**, and that of *p*-methoxy-phenyl azide **43**, a strong nucleophilic azide, with electrophilic acrylonitrile **40** were studied (see Scheme S2).



Scheme S2. 32CA reactions of *p*-nitro-phenyl azide **42** with enol ether **26** and *p*-methoxy-phenyl azide **43** with acrylonitrile **40**.

Analysis of the CDFT indices indicates that while *p*-nitro-phenyl azide **42** is the most electrophilic species of the substituted azides given in Table S1, ω = 2.66 eV, *p*-methoxy-phenyl azide **43** is the most nucleophilic one, *N* = 3.47 eV. Consequently, it is expected that **42** participates in polar 32CA reactions towards nucleophilic ethylenes such as enol ether **26**, *N* = 3.27 eV, and **43** with electrophilic ethylenes such as acrylonitrile **40**, ω = 1.74 eV (see Table S2).

The total electronic and relative energies of the stationary points involved in the two 32CA reactions are given in Table S3). The 32CA reaction of *p*-nitro-phenyl azide **42** with enol ether **26** presents an activation energy of 12.8 kcal·mol^{-1}, and a high *meta* regioselectivity as **TS-42-o** is located 6.3 kcal·mol^{-1} above **TS-42-m**. This 32CA reaction is exothermic by 32.8 kcal·mol^{-1}. Interestingly, despite the strong electrophilic activation of *p*-

nitro-phenyl azide **42**, the activation energy of this highly polar *zw-type* 32CA reaction is only 2.1 kcal·mol^{-1} lower than that of phenyl azide **6** (see Table 3 in the Manuscript). On the other hand, the 32CA reaction of *p*-methoxy-phenyl azide **43** with acrylonitrile **40** presents an activation energy of 16.6 kcal·mol^{-1}, the reaction being exothermic by 24.8 kcal·mol^{-1}. This 32CA reaction shows low *ortho* regioselectivity, as **TS-43-m** is located only 0.6 kcal·mol^{-1} above **TS-43-o**. Despite the strong nucleophilic activation of *p*-methoxy-phenyl azide **43**, the activation energy of this *zw-type* 32CA reaction decreases by only 0.6 kcal·mol^{-1} with respect to that of phenyl azide **6**.

Table S3. ωB97X-D/6-311G (d,p) gas phase total, E in a.u., and relative electronic energies, ΔE in kcal mol^{-1}, of the stationary points involved in the 32CA reactions of *p*-nitro-phenyl azide **42** with vinyl ether **26** and that of *p*-methoxy-phenyl azide **43** with acrylonitrile **40**. The GEDT computed at the TSs are given in an average number of electrons, e.

	E	ΔE	GEDT
26	-193.096926		
42	-600.275928		
TS-42-o	-793.342493	19.1	0.15
TS-42-m	-793.352478	12.8	0.28
CA-42-o	-793.425013	-32.7	
CA-42-m	-793.425074	-32.8	
40	-170.808643		
43	-510.302839		
TS-43-o	-681.085044	16.6	-0.06
TS-43-m	-681.084045	17.2	-0.03
CA-43-o	-681.151080	-24.9	
CA-43-m	-681.150549	-24.5	

The values of GEDT at the azide framework of the TSs are 0.15 e at **TS-42-o** and 0.28 e at **TS-42-m**, and −0.06 e at **TS-43-o** and −0.03 e at **TS-43-m** (see Table S3). Thus, while the 32CA reaction of nucleophilic azide **43** has a very low polar character, being classified as NEDF, that of electrophilic azide **42** has a very high polar character, being classified as REDF. Note that the GEDT at **TS-43-m** is only 0.03 e higher than that at **TS-26-m** (see Table 4 in the Manuscript). Consequently, only the electrophilic activation of phenyl azide **6** causes some acceleration of these *zw-type* 32CA reactions.

When the reaction rate constants of the 32CA reactions of substituted azides **42** and **43** are compared with respect to that of phenyl azide **6** with ethylene **5**, it is found that these

32CA reactions are accelerated by less than 20 times, showing the poor activation of these *zw-type* 32CA reactions of aryl azides (see Table S4).

Table S4. ωB97X-D/6-311G(d,p) enthalpies, H in a.u., entropies, S in cal mol^{-1} K^{-1}, Gibbs free energies, G in a.u., activation Gibbs free energies, $\Delta G^{\neq}$ in kcal mol^{-1}, and relative reaction rate constants, k_r, computed in toluene at 110 ºC, of the 32CA reactions of *p*-nitro-phenyl azide **42** with vinyl ether **26**, and that of *p*-methoxy-phenyl azide **43** with acrylonitrile **40**.

	H	S	G	$\Delta G^{\neq}$	k_r
42	-600.15687	108.238	-600.222953		
26	-193.00532	77.862	-193.052858		
TS-42-m	-793.14044	140.023	-793.225936	31.30	20.00
43	-510.15249	106.955	-510.217798		
40	-170.75383	69.096	-170.796016		
TS-43-o	-680.87889	133.742	-680.960554	33.42	1.23

What is the origin of the low electronic activation of the zw-type 32CA reactions of the substituted phenyl azides despite their high electrophilic and nucleophilic character?

In order to understand the low reactivity of substituted phenyl azides, the Parr functions of electrophilic *p*-nitro-phenyl azide **42** and the nucleophilic *p*-methoxy-phenyl azide **43** were analyzed. Figure S4 shows the electrophilic P_k^+ Parr functions of *p*-nitro-phenyl azide **42** and the nucleophilic Parr functions of *p*-methoxy-phenyl azide **43**.

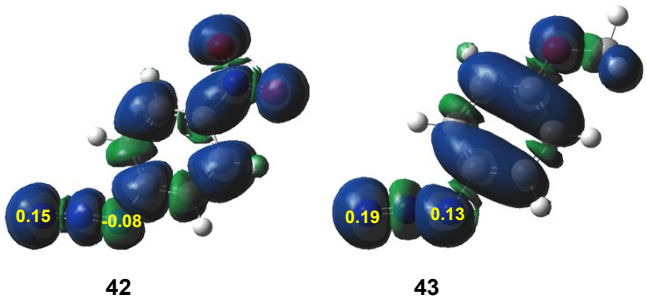


Figure S4. 3D representations of the Mulliken atomic spin densities of the radical anion of azide **42** and the radical cation of azide **43**, including the corresponding electrophilic P_k^+ and nucleophilic P_k^- Parr functions.

As can be observed, the aromatic ring of these aryl azides is the molecular region that is more electrophilically and nucleophilically activated (see Figure S4). The nitrogen nuclei present Parr functions lower than 0.20. Note that in methyl azide **44**, these nitrogen nuclei have Parr functions higher than 0.45 (see Figure S3). As the local electrophilicity ω_k and

nucleophilicity N_k indices are obtained by the product of the global index by the corresponding Parr functions,[7] low Parr function values imply a low local activation despite the global electronic activations. These findings account for the comparable reactivity of aryl azides and phenyl azide **6**.

*5. M06-2X/6-311G(d,p) calculations of the stationary points involved in the more favorable reaction paths of the 32CA reactions of phenyl azide **6** with supernucleophilic vinyl amine **22** and with strong electrophilic acrylonitrile **40***

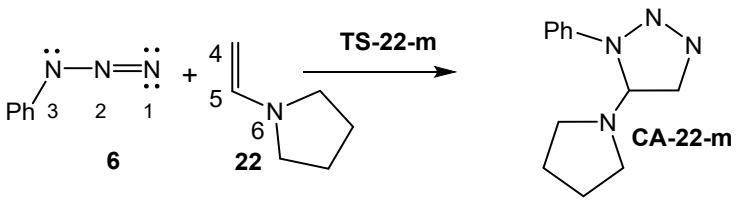
In order to investigate the dependency of the relative energies and GEDT values with the selected DFT functional, the TSs involved in the more favorable reaction pathways of the 32CA reactions of phenyl azide **6** with the supernucleophilic vinyl amine **22** and with the strong electrophilic acrylonitrile **40** were computed at the M06-2X/6-311G(d,p) computational level[26] (see Table S5). A comparison of the relative energies and GEDT values calculated with the two selected functionals at the more favorable **TS-22-m** and **TS-40-o** shows no appreciable changes (see Tables 3 and 4 in the Manuscript, and Table S5). While the changes in relative energies are less than 1.5 kcal·mol^{-1}, those in GEDT values are less than 0.02 e, showing that both functionals accurately describe the same polar processes.

Table S5. M06-2X/6-311G(d,p) gas phase total, E in a.u., and relative, ΔE in kcal mol^{-1}, electronic energies of the stationary points involved in the more favorable reaction paths of the 32CA reactions of phenyl azide **6** with supernucleophilic vinyl amine **22** and with strong electrophilic acrylonitrile **40**. The GEDT computed at the TSs is given in average number of electrons, e.

	E	ΔE	GEDT
6	-395.7684407		
22	-289.9198382		
TS-22-m	-685.6705022	11.2	-0.36
CA-22-m	-685.7325484	-27.8	
40	-170.8006321		
TS-40-o	-566.5420498	17.0	0.05
CA-40-o	-566.6085145	-24.8	

*6. Bonding Evolution Theory (BET) study of the [3+2] cycloaddition (32CA) reaction of phenyl azide **6** with vinyl amine **22***

In order to characterize the mechanism type of the 32CA reactions of aryl azides, a Bonding Evolution Theory[27] (BET) study of the more favorable *meta* regioisomeric reaction path associated with the 32CA reaction of phenyl azide **6** with vinyl amine **22** was performed (see Scheme S3). The populations of the most significant valence basins, among other relevant parameters, of the selected structures of the IRC are gathered in Table S6.



Scheme S3. More favorable *meta* regioisomeric reaction path associated with the 32CA reaction of phenyl azide **6** with vinyl amine **22**.

The polar 32CA reaction of phenyl azide **6** with vinyl amine **22** takes place along nine phases (see Table S6). The topological features of the ELF of the first point of the IRC, structure **S1**, show significant similarity to those shown in section 2.1 for phenyl azide **6**. At the same time, the ELF topology associated with the C4–C5 bonding region of vinyl amine **22**, which integrates a total population of 3.53e [V(C4,C5) and V'(C4,C5)], agrees with the double bond character of this region of ethylene **22**.

At the beginning of *Phase I*, the population of the N1–N2 bond region slightly increases by 0.10 e, while N2–N3 and C4–C5 bonding regions are marginally depopulated by 0.09e and 0.30e [see V(N1,N2), V(N2,N3), V(C4,C5), V'(C4,C5) at structure **S2** in Table S6]. This change is interesting, taking into account that the N1-N2 multiple bond region has to be depopulated to a single bond at the dihydro triazole **CA-22-m** (see Scheme S3). The non-bonding electron density at the N1 and N3 nitrogens are kept at 3.74 e and 3.37 e, respectively.

At the start of *Phase III*, because of a strong depopulation of the N1–N2 bonding region by 0.74 e, and the slight depopulation of the N2–N3 bonding region by 0.9e, a non-bonding electron density region at the N2 nitrogen, integrating 0.85e [V(N2)], is created. The population of this non-bonding electron density region, which has been associated with the N2 lone pair present in the Lewis structure of **CA-22-m**, increases along the IRC path to

reach a population of 2.80 e at **S11** (see Table S6). Minor electron density changes are observed in the C4–C5 bonding region of the ethylene framework.

At the beginning of *Phase IV*, the populations of the N1–N2 and N2–N3 bonding regions decrease by 0.63 e and 0.32 e, respectively, while that of the N2 non-bonding electron density is strongly increased by 0.96 e, to reach 1.81 e at **S4**. On the other hand, the C4-C5 bonding region has been depopulated by 0.15 e.

In *Phase V*, the population of N1–N2 and N2–N3 bond regions have decreased by 0.33 e and 0.17e, respectively, while that of the N3 non-bonding region has increased by 0.53 e to reach 1.81e. Interestingly, a non-bonding electron density region at the C4 carbon, with an initial population of 0.36 e [V(C4)] is created (see Table S6). The electron density of this non-bonding region comes from the depopulation of the C4–C5 bonding region, which has been depopulated by 0.56 e [V(C4,C5)]. The structure of **S5** corresponds with that of **TS-22-m**. From **S1**, the energy cost to reach this TS is 15.4 kcal·mol^{-1}.

In *Phase VI*, the non-bonding electron density region of the N1 nitrogen has been increased by 0.08 e. This behavior causes the V(N1) monosynaptic basin present at **S5** to split into two monosynaptic basins [V(N1) and V'(N1)] at **S6**. At this structure, the population of the non-bonding region present at C4 has increased by 0.16 e [V(C4)], while that of the C4–C5 bonding region has decreased by 0.21 e [V(C4,C5)].

In *Phase VII*, the first and most relevant topological change along the IRC is observed. At structure **S7**, while one of the two V(N1) monosynaptic basins and the C4 *pseudoradical* center[28] present in **S6** have disappeared, the formation of the first N1–C4 single bond is observed at an N1–C4 distance of 1.685 Å, and with an initial population of 1.17 e [V(N1,C4)] (see Table S6). Consequently, the N1–C4 single bond is formed by sharing the C4 non-bonding electron density and some of the N1 nitrogen.

The only topological change observed at **S8** is the split of the non-bonding electron density present at the N3 nitrogen into two monosynaptic basins [V(N3) and V'(N3)]. The recently created N1–C4 single bond has reached a population of 1.62 e [V(N1,C4)] at the beginning of *Phase VIII*.

At the beginning of *Phase IX*, the second most relevant topological change along the IRC is observed. At structure **S9**, the formation of the second N3–C5 single bond is observed at an N3–C5 distance of 1.873 Å and with an initial population of 1.24 e [V(N3,C5)] (see Table S6). This new N3–C5 single bond is mainly formed by donating some N3 non-bonding

electron density to the C5 carbon. At the end of this last phase, the new N1−C4 and N3−C5 single bonds have reached a population of 1.76 and 1.63 e, respectively.

Formation of the second N3−C5 single bond begins when the first N1−C4 single bond has reached a population of 1.69 e, i.e., a 96 % of its final population. Consequently, this 32CA reaction takes place via a non-concerted *two-stage one-step* mechanism.[29]

Table S6. ELF valence basin populations, distances of the forming bonds, GEDT, IRC values, and relative[a] electronic energies of the IRC structures **S1** – **S10** defining the nine phases characterizing the molecular mechanism of the 32CA reaction between phenyl azide **6** and with vinyl amine **22**. Distances are given in angstroms, Å, electron populations, and GEDT values in the average number of electrons, e, and relative energies in kcal·mol^{-1}.

Structures	**S1**	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**	**S10**
Phases	*I*	*II*	*III*	*IV*	*V*	*VI*	*VII*	*VIII*	*IX*	
d1 (N1-C4)	3.409	2.928	2.737	2.349	1.966	1.823	1.685	1.502	1.486	1.474
d2(N3-C5)	3.238	2.859	2.784	2.650	2.526	2.481	2.429	2.056	1.873	1.485
GEDT	0.00	0.00	0.00	0.09	0.34	0.48	0.58	0.60	0.53	0.38
ΔE	0.0	2.6	4.7	11.3	15.4	14.2	11.60	2.06	-2.4	-20.9
V(N1,N2)	2.44	4.27	3.53	2.90	2.57	2.45	2.35	2.29	2.33	2.39
V'(N1,N2)	1.73									
V(N2)			0.85	1.81	2.34	2.47	2.57	2.70	2.73	2.80
V(N2,N3)	2.46	2.37	2.28	1.96	1.79	1.80	1.80	1.74	1.68	1.53
V(C4,C5)	1.80	1.71	1.70	3.32	2.76	2.55	2.39	2.19	2.11	1.98
V'(C4,C5)	1.73	1.79	1.77							
V(C5,N6)	1.96	1.99	2.01	2.61	2.62	2.65	2.68	2.57	2.39	1.82
V(N1)	3.75	3.74	3.73	3.73	3.88	3.67	3.52	3.25	3.16	2.99
V'(N1)						0.29				
V(C4)					0.36	0.52				
V(N1,C4)							1.17	1.62	1.69	1.76
V(N3)	3.38	3.37	3.37	3.4	3.47	3.46	3.47	1.45	1.60	1.16
V'(N3)								2.06	0.89	1.23
V(N3,C5)									1.24	1.63
V(N3,CPh)	1.84	1.87	1.88	1.93	1.96	1.96	1.96	1.89	1.85	1.85

7. Computational Details

The *ω*B97X-D[30] functional, including long-range exchange and semi classical London dispersion corrections, has demonstrated to describe kinetics, GEDT, and covalent processes more accurately than the B3LYP functional.[31,32] The *ω*B97X-D has shown to be an efficient functional in the study of organic reactions.[33] The standard 6-311G(d,p)[34] basis set, which includes d-type polarization for second-row elements and p-type polarization functions for hydrogens, was used throughout this MEDT study. The TSs involved in the more favorable reaction pathways of the 32CA reactions of phenyl azide **6** with ethylenes **22** and **40** were also computed using the M06-2X functional.[26] The TSs were characterized by the presence of only one imaginary frequency. The Berny method was used in optimizations.[35,36] The intrinsic reaction coordinates (IRC) paths[37] were traced to obtain the energy profiles connecting each TS to the two associated minima in the potential energy surface using the Hratchian-Schlegel Hessian-based Predictor-Corrector integrator.[38-40]

Solvent effects of toluene in the thermodynamic calculations were taken into account by full optimization of the gas-phase structures at the same computational level using the polarizable continuum model[41,42] (PCM) in the framework of the self-consistent reaction field[43-45] (SCRF). Values of *ω*B97X-D /6-311G(d,p) enthalpies, entropies, and Gibbs free energies in toluene were calculated with standard statistical thermodynamics at 110 ºC and 1 atm[5] by PCM frequency calculations at the solvent-optimized structures.

The GEDT[20] values were computed using the equation GEDT(f) = Σq_f, where q are the natural charges[4,5] of the atoms belonging to one of the two frameworks (f) at the TS geometries. Reactivity indices[6,7] were calculated using the equations in reference 7. It is worth mentioning that within the Kohn-Sham[46] DFT approach to the electronic problem, MOs are purely instrumental in determining electron density, which is the fundamental variable.[47] Using Koopmans theorem[48] and the Kohn-Sham formalism,[46] the ionization potential (I) and the electron affinity (A) of an atom or molecule used to calculate the global reactivity indices are approximated by the HOMO and LUMO energies.[6,7]

The Gaussian 16 suite of programs was used to perform the calculations.[49] ELF[1] analyses of the *ω*B97X-D/6-311G(d,p) monodeterminantal wavefunctions were done by using the TopMod[50] package with a cubical grid of step size of 0.1 Bohr. Molecular geometries and ELF basin attractors were visualized by using the GaussView program.[51]

A stand-alone script based on the Ramer-Douglas-Peucker algorithm[52,53] was used to find a reduced but still suitable number of points on which to run the Interacting Quantum Atoms[54] (IQA) - relative energy gradient[55] (REG) analysis, out of the 242 (vinyl amine 22) or 301 (acrylonitrile 40) points belonging to the respective activation IRC paths; an RMSE value of 0.05 kcal·mol^{-1} was considered (see Section 8 for more information). The IQA analysis was performed with the AIMAll package[56] using the corresponding M06-2X/6-311G(d,p) monodeterminantal wavefunctions. The REG analysis was carried out via the in-house program REG.py.[57]

8. Theoretical background on Relative Energy Gradient (REG) - Interacting Quantum Atoms (IQA)

The IQA scheme divides the total energy into two main energy contributions: the intra-atomic energy, E_{intra}^{A}, and the interatomic energy, V_{inter}^{AB}.[54] The interatomic energy is, in turn, divided into two additional terms: the interatomic electrostatic energy (typically referred to as "classical"), V_{cl}^{AB}, and the interatomic exchange-correlation energy, V_{xc}^{AB}, in such a way that $V_{inter}^{AB} = V_{cl}^{AB} + V_{xc}^{AB}$. While E_{intra} has been associated with steric effects,[58] V_{cl} is related to electrostatic interactions,[50,60] and V_{xc} quantifies covalency.[61] Given that plain V_{inter}^{AB} terms should not be used as covalent-bond strength descriptors,[62] chemical graphs thus being related only to V_{xc}^{AB}, the REG analyses have been performed on a full IQA partitioning, delivering both V_{xc}^{AB} and V_{cl}^{AB}. The REG method[55] compares the gradient of a given energy contribution E_i against the gradient of the total energy E_{total}, using linear regression: $E_i(s) = m_{REG,i}E_{total}(s) + c_i$, where s is the control coordinate (IRC in our case) governing the change in the system, $m_{REG,i}$ is the REG value itself, and c_i is the y-intercept, which has currently no known chemical meaning. Thus, the REG method is only valid when the Pearson correlation coefficient R is close to 1 (these values for the studied reactions are given in Table S7). The REG values allow a semi-quantitative interpretation of the individual energy terms contributions to the total energy. Both the sign and the magnitude of the REG value are important. In summary, (energy) terms E_i with large positive REG_i values contribute the most to the total behaviour of the system, while terms with large negative REG_i values work against the total behaviour of the system. For instance, in the activation energy path, energy terms with positive REG values are unfavourable and contribute to the barrier, while those with negative REG values are favourable and facilitate the reaction. Ranking the energies from largest to smallest produces an ordered list of IQA energy terms that directly contribute towards (or against) a given energy segment, which in our case coincides with a barrier. This list provides a chemically intuitive interpretation for each energy segment being considered.

9. The Ramer-Douglas-Peucker (RDP) algorithm

The RDP algorithm[52] is a method that is mainly used in image processing and cartography to cut down the number of points of polylines (i.e., lines defined by multiple segments) while maintaining a reasonable graphic resolution of the image. In the context of potential energy surfaces, this algorithm can be used to consider the minimal number of points on which to run the REG-IQA analysis, thereby reducing its computational cost, while obtaining chemically meaningful results.

The RDP algorithm is heuristic because it defines the number of points through a cut-off parameter usually named ε, which is dimensionless. When applied to potential energy surfaces, it is then helpful to translate the parameter to a more meaningful metric such as an RMSE, which is expressed in units of energy. This is carried out by a mixture of recursive cross-validation and linear interpolation. Thus, the algorithm outputs the number of most suitable points to consider along the activation energy path given a specific RMSE of tolerance.

For instance, applied to the activation IRC paths of the 32CA reactions of phenyl azide **6** with vinyl amine **22** and acrylonitrile **40**, the RDP algorithm yielded only 11 and 14 geometries, respectively, out of a total of 242 and 301 with an RMSE of confidence value of 0.05 kcal·mol^{-1} (see Figure S5). This represents a substantial reduction in the number of geometries, which saves much computation time given the high cost of IQA calculations.

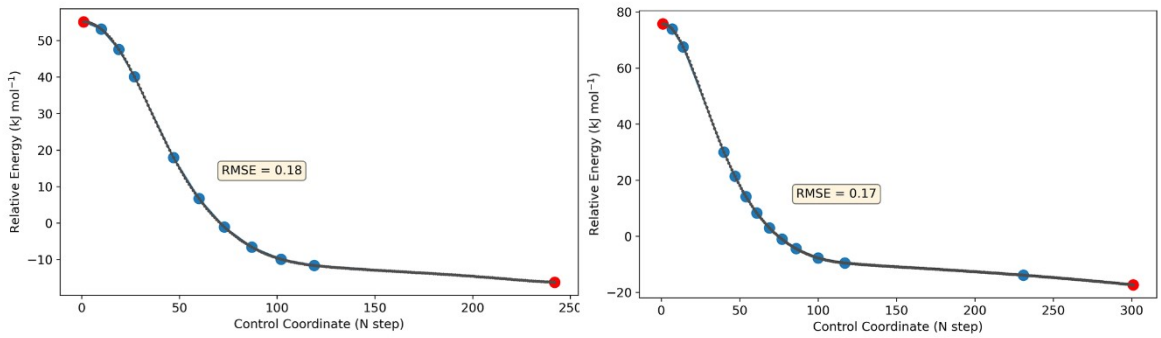


Figure S5. Most suitable geometries to represent the full activation IRC paths of the 32CA reactions of phenyl azide **6** with a) vinyl amine **22** and b) acrylonitrile **40**, with an RMSE value of 0.05 kcal·mol^{-1}.

Table S7. REG_i values of the total E_{IQA}^{A} energy terms and ΔE_{IQA}^{A} energy differences from the TS to the first structure of the reaction path, in kcal·mol^{-1}, for the main atoms participating in the 32CA reactions of phenyl azide **6** with vinyl amine **22** and acrylonitrile **40**.

	vinyl amine **22**		acrylonitrile **40**	
Energy term	REG	ΔE_{IQA}^{A}	REG	ΔE_{IQA}^{A}
E_{IQA}(N1)	-0.52	-12.8	-0.02	-1.7
E_{IQA}(N2)	0.43	6.5	0.46	9.7
E_{IQA}(N3)	-0.32	-7.1	-0.07	-3.3
E_{IQA}(C3')	-0.30	-5.3	0.00	0.4
E_{IQA}(C4)	0.44	8.2	0.26	6.8
E_{IQA}(C5)	0.93	20.2	0.15	3.9
E_{IQA}(X5')	-0.41	-7.6	-0.08	-1.9

Table S8. Twelve fully-partitioned IQA energy terms with the largest REG_i values and their energy differences from TSs to the first structures of the reaction paths, ΔE in kcal·mol^{-1}, for the 32CA reaction of phenyl azide **6** with supernucleophilic vinyl amine **22** and strongly electrophilic acrylonitrile **40**. Additional relevant data are given at the bottom.

vinyl amine **22**			acrylonitrile **40**		
Energy term	REG	ΔE	Energy term	REG	ΔE
V_{xc}(N1,N2)	3.20	67.6	V_{xc}(C4,C5)	2.14	53.5
V_{xc}(C4,C5)	2.59	53.9	V_{cl}(N1,N2)	1.57	33.7
V_{cl}(N1,N2)	1.91	26.7	E_{intra}(N3)	1.50	34.7
V_{xc}(N2,N3)	1.72	29.0	V_{xc}(N1,N2)	1.29	33.5
V_{cl}(N1,N5')	1.63	35.5	V_{xc}(N2,N3)	1.29	31.9
E_{intra}(C5)	1.50	33.3	E_{intra}(C4)	0.71	17.1
V_{xc}(N3,C3')	-0.79	-14.5	V_{cl}(N1,C5')	-0.44	-11.4
V_{cl}(N2,N5')	-0.95	-20.3	V_{cl}(N3,C3')	-0.63	-13.6
V_{cl}(N3,C5)	-1.10	-24.1	V_{cl}(N2,NC)	-0.64	-15.1
V_{cl}(C5,N5')	-2.66	-56.7	E_{intra}(N2)	-1.61	-39.5
E_{intra}(N2)	-2.73	-51.3	V_{xc}(N1,C5)	-1.66	-41.5
V_{xc}(N1,C4)	-3.45	-71.7	V_{xc}(N3,C4)	-2.40	-59.5
E_{intra}(N3)	0.69	14.6	V_{xc}(N3,C3')	-0.07	-1.5
V_{cl}(N3,C3')	-0.56	-9.6	V_{cl}(C5,C5')	-0.07	-1.1
E_{intra}(N1)	-0.76	-14.3	E_{intra}(N1)	-0.31	-7.8

Table S9. Pearson correlation coefficients *R* of the twelve IQA terms with largest REG_i values and other relevant energy terms, along the activation IRC path associated with the *zw-type* 32CA reactions of phenyl nitrone **6** with vinyl amine **22** and acrylonitrile **40**.

vinyl amine **22**		acrylonitrile **40**	
Energy term	R	Energy term	R
V_{xc}(N1,N2)	0.91	V_{xc}(C4,C5)	0.95
V_{xc}(C4,C5)	0.92	V_{cl}(N1,N2)	0.98
V_{cl}(N1,N2)	0.99	E_{intra}(N3)	0.97
V_{xc}(N2,N3)	0.96	V_{xc}(N1,N2)	0.94
V_{cl}(N1,N5')	0.95	V_{xc}(N2,N3)	0.90
E_{intra}(C5)	0.92	E_{intra}(C4)	0.99
V_{xc}(N3,C3')	-0.98	V_{cl}(N1,C5')	-0.92
V_{cl}(N2,N5')	-0.98	V_{cl}(N3,C3')	-0.74
V_{cl}(N3,C5)	-0.96	V_{cl}(N2,NC)	-0.98
V_{cl}(C5,N5')	-0.88	E_{intra}(N2)	-0.95
E_{intra}(N2)	-0.97	V_{xc}(N1,C5)	-0.96
V_{xc}(N1,C4)	-0.94	V_{xc}(N3,C4)	-0.98
E_{intra}(N3)	0.81	V_{xc}(N3,C3')	-0.99
V_{cl}(N3,C3')	-0.62	V_{cl}(C5,C5')	-0.83
E_{intra}(N1)	-0.95	E_{intra}(N1)	-0.87

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Table S10. ωB97X-D/6-311G(d,p) Total electronic energies, in a.u., of the stationary points involved in the 32CA reactions of phenyl azide **6**.

18	-406.699994	**TS-18-o**	-802.458209	**CA-18-o**	-802.538559
		TS-18-m	-802.475958	**CA-18-m**	-802.534509
19	-446.016705	**TS-19-o**	-841.770088	**CA-19-o**	-841.850248
		TS-19-m	-841.789095	**CA-19-m**	-841.846433
20	-266.699656	**TS-20-o**	-662.442332	**CA-20-o**	-662.528038
		TS-20-m	-662.470337	**CA-20-m**	-662.525547
21	-422.702342	**TS-21-o**	-818.463156	**CA-21-o**	-818.548706
		TS-21-m	-818.478352	**CA-21-m**	-818.540400
22	-289.967291	**TS-22-o**	-685.731105	**CA-22-o**	-685.814329
		TS-22-m	-685.737424	**CA-22-m**	-685.798367
23	-481.895395	**TS-23-o**	-877.654177	**CA-23-o**	-877.735299
		TS-23-m	-877.670509	**CA-23-m**	-877.730778
24	-212.547628	**TS-24-o**	-608.300295	**CA-24-o**	-608.378731
		TS-24-m	-608.315413	**CA-24-m**	-608.379967
26	-193.096927	**TS-26-o**	-588.850947	**CA-26-o**	-588.932933
		TS-26-m	-588.859284	**CA-26-m**	-588.933345
28	-272.711798	**TS-28**	-668.477259	**CA-28**	-668.565801
30	-195.312129	**TS-30**	-591.074204	**CA-30**	-591.155288
31	-234.632667	**TS-31**	-630.389104	**CA-31**	-630.467314
34	-345.764878	**TS-34-o**	-741.524004	**CA-34-o**	-741.596121
		TS-34-m	-741.527565	**CA-34-m**	-741.594016
37	-306.446664	**TS-37-o**	-702.207597	**CA-37-o**	-702.276824
		TS-37-m	-702.211094	**CA-27-m**	-702.278612
39	-305.177897	**TS-39-o**	-700.936317	**CA-39-o**	-701.087488
		TS-39-m	-700.938337	**CA-39-m**	-701.082750
40	-170.808643	**TS-40-o**	-566.567301	**CA-40-o**	-566.634371
		TS-40-m	-566.565754	**CA-40-m**	-566.634397
41	-533.037151	**TS-41**	-928.798610	**CA-41**	-928.942747
15	-283.068767	**TS-15-o**	-678.831833	**CA-15-o**	-678.901201
		TS-15-m	-678.830312	**CA-15-m**	-678.905548

Table S11. ωB97X-D/6-311G(d,p) Total, E in a.u, and relative, ΔE in kcal mol^{-1}, energies of the stationary points involved in the 32CA reactions of simplest azide **8**, methyl azide **44**, and phenyl azide **6** with ethylene **5**. The GEDT computed at the TSs is given in average number of electrons, e.

	E	ΔE	GEDT
5	-78.579526		
8	-164.76534		
TS-8	-243.31396	19.4	-0.04
CA-8	-243.38844	-27.3	
44	-204.06845		
TS-44	-282.61949	17.9	-0.02
CA-44	-282.69992	-32.6	
6	-395.78609		
TS-6	-474.33716	17.9	-0.07
CA-6	-474.41607	-31.7	

Table S12. ωB97X-D/6-311G(d,p) Total electronic energes, E in a.u., enthalpies, H in a.u., entropies, S in cal mol^{-1} K^{-1}, activation Gibbs free energies, ΔG in a.u., and relative activation Gibbs free energies, $\Delta G^{\neq}$ in kcal·mol^{-1}, computed in toluene at 110 ºC, of the selected 32CA reactions of phenyl azide **6**.

	E	H	S	G	$\Delta G^{\neq}$
6	-395.78808	-395.67151	91.531	-395.727400	
5	-78.580149	-78.523532	55.034	-78.557135	
TS-5	-474.33934	-474.16506	108.036	-474.231023	33.58
18	-406.70124	-406.45676	106.391	-406.521724	
TS-18-m	-802.47932	-802.11732	152.766	-802.210601	24.17
19	-446.01786	-445.74201	112.05	-445.810425	
TS-19-m	-841.79263	-841.39926	160.089	-841.497008	25.61
21	-422.70476	-422.47177	104.477	-422.535566	
TS-21-m	-818.48248	-818.13204	151.565	-818.224588	24.08
23	-481.89781	-481.64665	111.271	-481.714588	
TS-23-m	-877.67484	-877.30619	157.883	-877.402588	24.72
28	-272.71233	-272.54859	79.957	-272.597408	
TS-28	-668.47941	-668.19824	127.933	-668.276358	30.40
30	-195.31265	-195.18681	74.601	-195.232361	
TS-30	-591.07626	-590.83299	121.059	-590.906911	33.16
31	-234.63322	-234.47614	79.024	-234.524394	
TS-31	-630.3912	-630.11665	128.813	-630.195300	35.45
37	-306.44949	-306.34246	86.688	-306.395391	
TS-37-m	-702.21487	-701.99031	130.805	-702.070175	33.02
39	-305.18136	-305.09872	84.646	-305.150408	
TS-39-o	-700.94142	-700.74149	136.896	-700.825081	33.09
40	-170.81224	-170.75383	69.095	-170.796015	
TS-40-o	-566.573	-566.39698	118.448	-566.469299	33.96
41	-533.04183	-532.90851	115.824	-532.979225	
TS-41	-928.80492	-928.55438	163.613	-928.654281	30.07
15	-283.07236	-283.00863	75.073	-283.054469	
TS-15-o	-678.83688	-678.65554	123.503	-678.730944	31.96

ωB97XD/6-311G(d,p) gas phase computed total energies, single imaginary frequency, and Cartesian coordinates of the stationary points involved in the 32CA reactions of phenyl azide **6** with the selected 18 ethylene derivatives.

6
E = -395.786087 a.u.

N -3.32549700 -0.54697400 -0.00073900
N -2.39816300 0.09162500 -0.00008800
N -1.46945100 0.89608000 0.00069900
C 0.88107900 1.30494900 -0.00006300
C 2.19855700 0.87471700 -0.00034500
C 2.49706300 -0.48397300 -0.00024900
C 1.46361600 -1.41157800 0.00011800
C 0.13934400 -0.99309800 0.00041700
C -0.15163000 0.36999200 0.00034400
H 0.63194400 2.35897400 -0.00020700
H 2.99805300 1.60658800 -0.00065400
H 3.52811800 -0.81657800 -0.00047400
H 1.68466100 -2.47271300 0.00018000
H -0.65917100 -1.72743500 0.00072700

18
E = -406.699994 a.u.

C 0.69879500 0.07062200 -0.07867400
C 1.47892500 1.16563500 -0.04699800
C -1.44342700 -1.18394600 0.11263300
C -2.86456700 -0.73755700 -0.21709600
C -2.88168300 0.71275000 0.27802200
C -1.46587700 1.22214200 -0.02677200
N -0.66746600 0.01455300 -0.15859400
H -1.10985100 -2.01843600 -0.50907400
H -3.01731800 -0.77134500 -1.29967400
H -3.05895600 0.73061200 1.35726900
H -1.08051400 1.86068900 0.77969100
C 1.52687200 -1.19423300 -0.11835700
C 2.93042400 -0.69858700 0.26863000
H 1.15628000 -1.96880900 0.55932400
C 2.94097800 0.80199000 -0.08667500
H 1.12215800 2.18678700 -0.08358900
H 3.72698200 -1.26211300 -0.22165500
H 3.36842800 0.96875400 -1.08553600
H -1.37086400 -1.49761000 1.16695600
H -3.62410600 -1.36179300 0.25643200
H -3.65599100 1.31802200 -0.19544400
H -1.42337000 1.80803500 -0.95383000
H 1.50400400 -1.61691500 -1.13118400
H 3.06147600 -0.81155300 1.34839500
H 3.55127300 1.38091100 0.61380100

TS-18-o
E = -802.458209 a.u.
Freq = 457.53i cm^{-1}

N -0.85964400 -0.71634600 0.26610400
N -0.27651400 -0.43741400 1.37375500
N 0.71421800 0.11372500 1.64421200
C 1.46382800 0.77508400 -0.34529700
C 0.29172800 0.50997300 -1.06019900
C 3.71569400 0.27262700 0.49177100
C 4.67482500 -0.87256000 0.19172900
C 3.71651200 -2.03990200 -0.06133800
C 2.53215700 -1.38787400 -0.78697500
N 2.62226600 0.03332800 -0.44431600
H 4.16217300 1.25605700 0.32388800
H 5.25218900 -0.64875100 -0.71022700
H 3.38168700 -2.45191000 0.89470500
H 1.57518700 -1.81220000 -0.46118500
C 1.51913200 2.24236100 0.02659000
C 0.05292100 2.67897500 -0.08578300
H 1.94475400 2.42018300 1.01600300
C -0.52265800 1.77301900 -1.18692700
H 0.24145300 -0.26377800 -1.81365600
H -0.05726200 3.74129200 -0.30912800
H -0.34436900 2.21394000 -2.17714900
H 3.36534200 0.22646200 1.53328100
H 5.37323900 -1.05986400 1.00872800
H 4.16552300 -2.85076000 -0.63684400
H 2.59911700 -1.51785400 -1.87376200
H 2.14440000 2.76625200 -0.70890500
H -0.46038400 2.48208500 0.85918600
H -1.60117300 1.61704100 -1.09723300
C -2.25935000 -0.65412800 0.20698300
C -2.85066100 -1.05207300 -0.99447500
C -3.06421200 -0.16195700 1.23842500
C -4.22246300 -0.94646700 -1.16396000
H -2.21989300 -1.44092400 -1.78518900
C -4.43804500 -0.07824000 1.06320000
H -2.60902300 0.13877200 2.17481800
C -5.02510200 -0.46238300 -0.13666200
H -4.66887600 -1.25429400 -2.10280700
H -5.05409500 0.29631800 1.87306400
H -6.09810200 -0.38984100 -0.26836100

TS-18-m
E = -802.475958 a.u.
Freq = 335.64i cm^{-1}

N -0.82870100 -1.57946700 -1.80571600
N 0.18928900 -1.23289700 -1.33020200
N 0.54914200 -0.63567800 -0.25924600
C -2.00950400 -0.23482400 0.32862000
C -2.42056600 -1.16564800 -0.62738200
C -1.16205100 1.92499300 1.08625200
C -1.17593600 3.29590200 0.42111600

C -1.08885500 2.93860100 -1.06491700
C -1.96013900 1.68556400 -1.18263500
N -1.90921400 1.08722600 0.15384500
H -1.62122400 1.91698000 2.07696300
H -2.11600500 3.81238600 0.63748900
H -0.05586100 2.69066100 -1.32271800
H -1.57583200 0.98159800 -1.92536400
C -1.84406700 -0.88684300 1.67828100
C -1.83142700 -2.38273300 1.33691300
H -0.95567900 -0.55625300 2.21548000
C -2.68831200 -2.48476300 0.06354500
H -3.00007300 -0.86274100 -1.48949400
H -2.20035700 -3.00453200 2.15414300
H -3.75232500 -2.57960700 0.31814000
H -0.13614600 1.53725600 1.16586500
H -0.35306700 3.92637500 0.75920000
H -1.42205200 3.74108000 -1.72386400
H -2.99628400 1.92730400 -1.44435100
H -2.72312900 -0.62912200 2.28576500
H -0.80515200 -2.68294700 1.11263300
H -2.42105100 -3.34309200 -0.55684100
C 2.35480300 0.04089900 1.14289200
C 3.69648700 0.29888100 1.38066100
C 4.64264500 0.09179000 0.38338600
C 4.22441600 -0.37954800 -0.85610700
C 2.88422100 -0.63695600 -1.10478200
C 1.92826700 -0.42856300 -0.10355100
H 1.61834900 0.18547300 1.92581900
H 4.00535100 0.65937700 2.35588700
H 5.69101300 0.29263500 0.56964700
H 4.95056100 -0.54720900 -1.64432300
H 2.56544800 -1.00042100 -2.07459500

CA-18-o
E = -802.538558 a.u.

N -0.86852200 0.18214100 0.34613300
N -0.24219900 -0.10706700 1.51902500
N 0.96311700 0.17767700 1.50135900
C 1.37762400 0.68311300 0.14994500
C 0.03730000 0.76039700 -0.63178500
C 3.67938600 -0.18396200 0.17881000
C 4.31637700 -1.45177000 -0.37155400
C 3.15336700 -2.44466100 -0.30573100
C 1.92565200 -1.58948600 -0.65042000
N 2.34920600 -0.19133500 -0.43814900
H 4.22656900 0.72038400 -0.09881800
H 4.62750400 -1.29153400 -1.40813600
H 3.06086900 -2.83112200 0.71288000
H 1.07323400 -1.86527300 -0.01956700
C 1.86030500 2.13293000 0.28614800
C 0.57748800 2.96098400 0.20893000
H 2.42593900 2.27950500 1.20739600
C -0.22070600 2.25305000 -0.88983700

H 0.04968400 0.16158500 -1.54436700
H 0.76308000 4.01385900 -0.00960700
H 0.18214300 2.51585000 -1.87338200
H 3.62344600 -0.23019400 1.27636000
H 5.18694400 -1.77020900 0.20421000
H 3.27239900 -3.29611500 -0.97764100
H 1.62298500 -1.72628400 -1.69424000
H 2.50951400 2.36040300 -0.56507800
H 0.03711800 2.90887700 1.15949700
H -1.28506000 2.49506900 -0.88587100
C -2.19683600 -0.19132600 0.13661800
C -2.78320300 -0.00353400 -1.11750000
C -2.95483000 -0.75059100 1.17187400
C -4.10598500 -0.37274200 -1.32880300
H -2.21373300 0.43003300 -1.93001700
C -4.27146500 -1.11245800 0.94189400
H -2.49874200 -0.89702000 2.14110300
C -4.85989100 -0.92790800 -0.30573500
H -4.54527300 -0.22088000 -2.30836800
H -4.84620200 -1.54577400 1.75285700
H -5.89113900 -1.21328900 -0.47489300

CA-18-m
E = -802.534509 a.u.

N -1.96512300 -0.79822300 -1.87977800
N -0.82565700 -1.24054200 -1.66449800
N -0.36061900 -0.93059500 -0.41850900
C -1.22648100 0.11251700 0.23169500
C -2.44748800 -0.03795600 -0.71716800
C 0.23670800 1.81581800 1.34169700
C 0.83646800 3.12056200 0.83051100
C 1.01446700 2.82953900 -0.66087300
C -0.24178800 2.02695200 -1.01058900
N -0.67032800 1.42533800 0.25987100
H -0.31158700 1.94633900 2.27899900
H 0.12773300 3.94138800 0.97685600
H 1.90271200 2.20752400 -0.80755600
H -0.03417200 1.27121400 -1.77436400
C -1.73257900 -0.36315900 1.59962100
C -2.75821000 -1.43946700 1.25248300
H -0.93174400 -0.69952800 2.25893500
C -3.51710000 -0.81523900 0.07402700
H -2.82078200 0.92318600 -1.07153000
H -3.41012100 -1.68991500 2.09144900
H -4.26999400 -0.11532900 0.44793900
H 1.03507500 1.08136500 1.51440200
H 1.76933000 3.37715800 1.33496100
H 1.12244700 3.72831500 -1.27011800
H -1.03168500 2.67687700 -1.40584900
H -2.22843600 0.48399300 2.08404000
H -2.24849300 -2.35383600 0.93559600
H -4.02302000 -1.54380300 -0.56072100
C 1.50823700 -1.51812500 1.01683900

C 2.87337900 -1.59710600 1.25352400
C 3.77881700 -1.25006800 0.25787200
C 3.30706300 -0.83004300 -0.97988800
C 1.94275500 -0.72445100 -1.21344200
C 1.03413200 -1.05672300 -0.20997100
H 0.80371400 -1.82741800 1.77839000
H 3.23025400 -1.94995600 2.21441400
H 4.84467200 -1.32012400 0.44081900
H 4.00483300 -0.57254900 -1.76866100
H 1.57106700 -0.39504900 -2.17563900

19
E = -446.016705 a.u.

C -0.40255000 -0.04555900 -0.00527900
C -1.07551900 -1.18394400 -0.25189200
C 1.77225800 1.19184200 -0.14218100
C 3.20016500 0.65832200 -0.33066700
C 3.18403000 -0.69930900 0.37549400
C 1.77777200 -1.20380700 0.07332500
N 0.97542900 -0.00048000 0.14523600
H 1.43001500 1.70961900 -1.04613900
H 3.40372600 0.51413700 -1.39571000
H 3.30611900 -0.57148700 1.45496200
H 1.42040400 -1.94159400 0.79819000
C -1.12015000 1.26651800 0.22317300
C -2.59762600 1.20902800 -0.16151400
H -1.01377600 1.53638600 1.28202000
C -2.57855500 -1.28645900 -0.26657400
H -0.52722800 -2.10148300 -0.43450300
H -2.68883000 1.23002300 -1.25396300
H -2.93902500 -1.40304200 -1.29876000
H 1.71740000 1.90710900 0.68732400
H 3.95453400 1.34186100 0.06214000
H 3.96292000 -1.37614500 0.02036800
H 1.73438800 -1.67298200 -0.92508900
H -0.63035600 2.06497500 -0.34174200
H -3.11023300 2.09738500 0.21863800
H -2.89057500 -2.19492600 0.26091300
C -3.24554100 -0.06660100 0.36581000
H -4.32018800 -0.06937800 0.16157700
H -3.12299800 -0.10727600 1.45495100

TS-19-o
E = -841.770088
Freq = 454.31i cm^{-1}

N -0.83959400 -0.68862300 0.31695300
N -0.28280800 -0.38608000 1.43577900
N 0.71504000 0.17129100 1.67898300
C 1.52510300 0.68340300 -0.29158700
C 0.32488600 0.52000200 -1.00183900
C 3.66154300 -0.26046700 0.51647400

C 4.41970400 -1.52801100 0.14721800
C 3.28355500 -2.51067500 -0.13955600
C 2.21052200 -1.64228700 -0.80838500
N 2.53672400 -0.26633400 -0.41616200
H 4.27005400 0.63852800 0.39840600
H 5.01491400 -1.35552800 -0.75450300
H 2.89954100 -2.91118100 0.80291400
H 1.20611600 -1.92609400 -0.47815400
C 2.00183600 2.06418000 0.14092100
C 1.01993300 3.21019600 -0.14725300
H 2.24961900 2.03686200 1.20454800
C -0.61047100 1.67865200 -1.22185700
H 0.27469900 -0.27335700 -1.73651300
H 1.24546700 3.63838800 -1.13072800
H -0.40066000 2.11108700 -2.21065500
H 3.31537000 -0.30287000 1.55986300
H 5.08864700 -1.86234200 0.94179800
H 3.58623900 -3.35389900 -0.76228500
H 2.24048800 -1.73689200 -1.90086500
H 2.93740800 2.26152300 -0.39174300
H 1.17347100 4.00945100 0.58205500
H -1.64537600 1.32780900 -1.26017900
C -2.23702800 -0.72374800 0.23541000
C -2.78056900 -1.17872900 -0.96878000
C -3.09170000 -0.27578500 1.24737200
C -4.15383600 -1.17186300 -1.16088800
H -2.11201100 -1.53497600 -1.74397500
C -4.46456100 -0.29249300 1.05030700
H -2.67309600 0.06926600 2.18543600
C -5.00459400 -0.73242200 -0.15297700
H -4.56221100 -1.52334800 -2.10174000
H -5.11835000 0.04800000 1.84555000
H -6.07782200 -0.73741400 -0.30150400
C -0.43713400 2.75832500 -0.16095300
H -0.72855200 2.36971400 0.82019900
H -1.09261900 3.60584200 -0.37855000

TS-19-m
E= -841.789095 a.u.
Freq =338.78i cm^{-1}

N -0.74074100 -0.96719900 -2.09961300
N 0.30858200 -0.78251500 -1.59150400
N 0.68335700 -0.43342300 -0.41896300
C -1.79706700 -0.05262800 0.27255700
C -2.26007300 -0.79758400 -0.82328600
C -0.96316700 2.06238100 1.20668100
C -1.08489700 3.49625500 0.70764800
C -1.04094300 3.31885500 -0.81025600
C -1.83282300 2.03050300 -1.04437000
N -1.70446500 1.28964600 0.21448600
H -1.37583000 1.92381300 2.20741800
H -2.04428700 3.92186900 1.01700600
H -0.00671300 3.17597300 -1.13438600

H -1.42682400 1.44820200 -1.87436200
C -1.52882000 -0.70519100 1.60721300
C -1.45552900 -2.22354700 1.51011100
H -0.61247900 -0.30991300 2.04308500
C -2.68966300 -2.24911300 -0.67535600
H -2.80942100 -0.23831400 -1.57011900
H -1.39311900 -2.64766100 2.51573200
H -3.69139900 -2.36849300 -1.09826300
H 0.08673200 1.73193600 1.20772200
H -0.28803800 4.13487000 1.09009200
H -1.45473500 4.16563300 -1.35882900
H -2.89025000 2.23029700 -1.25329400
H -2.35295200 -0.41964500 2.27696300
H -0.53904600 -2.50004100 0.97834200
H -2.02875000 -2.87373800 -1.28606800
C 2.48489100 -0.08060500 1.09863200
C 3.83401700 0.00782500 1.40712100
C 4.79720400 -0.19609600 0.42575400
C 4.38762500 -0.49179300 -0.86990000
C 3.04073900 -0.58238200 -1.18850500
C 2.06725100 -0.37574900 -0.20346000
H 1.73425300 0.06869400 1.86704900
H 4.13448600 0.23536500 2.42419600
H 5.85137900 -0.12678700 0.66665400
H 5.12692400 -0.65395800 -1.64702400
H 2.72947500 -0.81137800 -2.20071600
C -2.67596000 -2.75529700 0.76789800
H -3.58039700 -2.41903300 1.29016400
H -2.69285400 -3.84823200 0.77691300

CA-19-o
E= -841.850248 a.u.

N -0.88101000 0.08420700 0.32499100
N -0.25273100 -0.14579300 1.51430000
N 0.95927500 0.09929100 1.47213800
C 1.37654800 0.52684600 0.09429900
C 0.05687400 0.45746500 -0.72468300
C 3.71612800 -0.27930400 0.14523800
C 4.35691800 -1.60335900 -0.24581300
C 3.20081800 -2.58242500 -0.04267300
C 1.98291300 -1.79161300 -0.53171200
N 2.37099400 -0.36807500 -0.43542700
H 4.25530600 0.58193300 -0.25628500
H 4.65768500 -1.57760900 -1.29767600
H 3.09391900 -2.80581900 1.02254800
H 1.10053300 -2.02236300 0.07426800
C 1.90155100 1.96104100 0.20583600
C 0.78675600 2.93596200 0.58452600
H 2.68507200 1.98823000 0.96530300
C -0.29100600 1.77279400 -1.41761900
H 0.12636300 -0.34079500 -1.46956500
H 1.20817800 3.93730300 0.69637400
H 0.48496400 1.94782200 -2.17035800

H 3.68389500 -0.18715000 1.24103100
H 5.23531100 -1.83816000 0.35758700
H 3.32854700 -3.52632800 -0.57514100
H 1.74545000 -2.04149600 -1.57200600
H 2.35982900 2.23597400 -0.74970200
H 0.40673100 2.65317800 1.56990700
H -1.23315900 1.67627200 -1.96216500
C -2.20389000 -0.33621900 0.15496200
C -2.71717600 -0.55824900 -1.12421800
C -3.03038300 -0.52580000 1.26819100
C -4.03866300 -0.95840000 -1.28371900
H -2.09019600 -0.43100900 -1.99747100
C -4.34119000 -0.93491000 1.09165900
H -2.62776600 -0.35866800 2.25787800
C -4.85908500 -1.14972900 -0.18233900
H -4.42197600 -1.12596700 -2.28399700
H -4.96912200 -1.08125100 1.96341300
H -5.88828100 -1.46237900 -0.31137000
C -0.36855400 2.94867600 -0.44199200
H -1.32653300 2.91605600 0.08294600
H -0.36180100 3.87815400 -1.01718600

CA-19-m
E= -841.846433 a.u.

N -1.14290000 -1.49898800 -1.89295500
N 0.05059400 -1.19304800 -1.74177100
N 0.29331700 -0.58598600 -0.54797600
C -0.96491800 -0.25718000 0.16711900
C -1.91106900 -1.15587200 -0.68450200
C -1.52466300 2.04740400 1.16556500
C -2.01837500 3.31060900 0.46145400
C -1.23702900 3.29137300 -0.85355000
C -1.21309600 1.80709300 -1.22411900
N -1.31203000 1.12979900 0.06112200
H -2.26163100 1.66742500 1.87899700
H -3.09109700 3.22618600 0.26323600
H -0.21547600 3.64469300 -0.68324500
H -0.29091400 1.53814200 -1.75162900
C -0.91032900 -0.72951900 1.62227200
C -0.47725400 -2.19425500 1.74935500
H -0.23534300 -0.09591700 2.20120100
C -2.33090500 -2.44670900 0.02299500
H -2.79259300 -0.58645400 -0.98459100
H -0.72667800 -2.53087300 2.75920600
H -3.10486400 -2.21288900 0.76194200
H -0.60808200 2.27179500 1.73927600
H -1.84981000 4.21187900 1.05336800
H -1.68313800 3.91264000 -1.63133500
H -2.05195700 1.54170400 -1.88449000
H -1.90804000 -0.59300600 2.04942000
H 0.61031100 -2.25482800 1.66261500
H -2.78280400 -3.11335400 -0.71519600
C 1.85365700 0.88698200 0.60522800

C 3.16187600 1.24438800 0.90791800
C 4.23168700 0.56240000 0.34712100
C 3.97847500 -0.49309200 -0.52316000
C 2.67997200 -0.87489900 -0.81778200
C 1.60202400 -0.18288100 -0.25461000
H 1.03352200 1.45276900 1.02150400
H 3.33913600 2.07605300 1.58077000
H 5.24997800 0.84907400 0.58114500
H 4.80284500 -1.03625200 -0.97157000
H 2.48308400 -1.69986100 -1.48913500
C -1.13462000 -3.11540400 0.69684000
H -1.44536700 -4.05627600 1.15663900
H -0.40654900 -3.37772000 -0.07592400

20
E= -266.699656 a.u.

C 0.82254200 -0.00000100 0.00000100
C -1.37413700 0.74397700 0.17010800
C -1.37413700 -0.74397700 -0.17011000
H -2.10762800 1.30651500 -0.41033500
H -1.57775700 -0.88845100 -1.24035900
H -1.57776300 0.88845100 1.24035500
H -2.10763000 -1.30651600 0.41033000
C 2.16233000 0.00000000 -0.00000200
H 2.71340100 0.91678800 -0.15602000
H 2.71340500 -0.91678600 0.15601500
N -0.01131600 -1.10589300 0.19495900
N -0.01131500 1.10589400 -0.19495600
H 0.34139700 -1.97784100 -0.16533500
H 0.34139800 1.97783800 0.16534800

TS-20-o
E = -662.442332 a.u.
Freq =491.21i cm^{-1}

N 0.55777000 0.12948100 -0.92719800
N -0.13386100 -0.93804600 -1.12384400
N -1.27106500 -1.16503900 -0.97617100
C -2.00334500 0.63699200 0.21452500
C -0.79560800 1.31795000 0.08190600
C -3.74394500 -0.58558100 1.16863400
N -2.38947600 -0.05703200 1.36524800
H -0.16769700 1.41279600 0.95817600
H -3.77826000 -1.67027300 1.28960700
H -0.74857800 2.12891300 -0.63124800
H -4.42608200 -0.13525400 1.89499200
N -3.16995800 0.93334800 -0.49557900
C -4.10253100 -0.16728000 -0.26657200
H -5.13517100 0.17354300 -0.35313600
H -3.93201800 -0.99428200 -0.96483000
H -3.01276700 1.17103200 -1.46296500

H -1.70738100 -0.72303100 1.68966800
C 1.86367500 0.00696400 -0.42438100
C 2.45469100 -1.21043300 -0.07347300
C 2.57670100 1.19412200 -0.23861100
C 3.73870300 -1.22909500 0.45189000
H 1.90984800 -2.13362500 -0.23002800
C 3.85190900 1.16286200 0.30476400
H 2.12036600 2.13311900 -0.52901100
C 4.44262100 -0.04723100 0.65082100
H 4.19091700 -2.17991800 0.71126100
H 4.39227400 2.09181100 0.44806800

TS-20-m
E = -662.470337 a.u.
Freq = 325.53i cm^{-1}

N 1.09865500 2.51557200 -0.02030800
N 0.14323000 1.82450000 -0.01933400
N -0.09797400 0.56215000 -0.01213000
C 2.65621100 0.16660200 0.00476800
C 2.81652800 1.55344000 -0.00399100
C 1.93774200 -1.89194900 -0.75667000
N 2.58622700 -0.62891100 -1.09285300
H 3.20257800 1.98798700 -0.91726500
H 0.92429200 -1.91799900 -1.16675600
C -1.80598100 -1.11686600 -0.02860000
C -3.13278900 -1.52202900 -0.02227900
C -4.15759100 -0.58423600 0.00469700
C -3.82971400 0.76713200 0.02516300
C -2.50608100 1.17970600 0.01968100
C -1.46661900 0.24023900 -0.00760900
H -1.01395000 -1.85671200 -0.05190200
H -3.36579100 -2.58132800 -0.03933900
H -5.19408200 -0.90010700 0.00955100
H -4.61591000 1.51434200 0.04642900
H -2.26203500 2.23511500 0.03635700
H 3.19085700 2.00052300 0.90811300
H 2.50697100 -2.73664800 -1.14827700
N 2.57574600 -0.61388800 1.11297800
C 1.90518400 -1.86849700 0.78942900
H 2.43117700 -2.71660800 1.23018500
H 0.87457600 -1.84924900 1.15535000
H 2.33302600 -0.15294600 1.97389800
H 2.34575400 -0.18358400 -1.96233900

CA-20-o
E = -662.528038 a.u.

N 0.42432800 0.19393000 -0.04152800
N -0.14964500 1.41715600 -0.02393200
N -1.39144900 1.37055000 0.00748500
C -1.86863500 -0.04939800 0.01404700
C -0.56188500 -0.86021200 0.05832300

C -4.06794700 -0.51325000 -0.71894900
N -2.68709300 -0.27944000 -1.16942100
H -0.51206300 -1.54850100 -0.78576000
H -4.78309000 -0.02295900 -1.38067900
H -0.46818800 -1.41033100 0.99883700
H -4.27815900 -1.58642600 -0.71915300
N -2.74248500 -0.31911200 1.13456900
C -4.09386900 0.03167900 0.70543700
H -4.83905900 -0.45337200 1.33914300
H -4.27340300 1.11556500 0.70062000
H -2.43879500 0.18313500 1.95924200
H -2.63724600 0.55122600 -1.74604200
C 1.81299500 0.04737500 -0.01945600
C 2.65419200 1.16400700 -0.05913300
C 2.36665200 -1.23263000 0.03604700
C 4.02753400 0.98694600 -0.04054100
H 2.21975900 2.15322600 -0.10245900
C 3.74699200 -1.39022700 0.05323900
H 1.72538600 -2.10496800 0.06397900
C 4.58619000 -0.28655200 0.01559200
H 4.67051900 1.85941400 -0.07095400
H 4.16352900 -2.39021200 0.09627500
H 5.66190400 -0.41382400 0.02910300

CA-20-m
E= -662.525547 a.u.

N 1.76651200 2.45406000 -0.08076100
N 0.56032300 2.21301300 -0.26021400
N 0.30381400 0.88537400 -0.43509900
C 1.48408900 0.06994800 -0.04823100
C 2.52511700 1.20154800 -0.10243000
C 1.95796600 -2.25155500 -0.13136300
N 1.69726400 -1.05833100 -0.92984700
H 3.10031100 1.17785400 -1.03463300
H 1.62292800 -3.15095700 -0.65244200
C -1.43981700 -0.73354000 -0.89358100
C -2.73768200 -1.19161600 -0.71655100
C -3.64285600 -0.47088600 0.05414100
C -3.23701700 0.71407700 0.65491800
C -1.93366300 1.16999400 0.50709900
C -1.03028900 0.44601600 -0.27066000
H -0.72979900 -1.27141500 -1.50784200
H -3.04830300 -2.11058300 -1.20100400
H -4.65898700 -0.82638100 0.17913000
H -3.93593500 1.28738600 1.25345600
H -1.61229400 2.09256900 0.97331800
H 3.21308700 1.15534100 0.74056200
H 3.01812700 -2.36850700 0.13200900
N 1.36948800 -0.53092000 1.27152200
C 1.13787200 -1.96383400 1.11716000
H 1.50195300 -2.51240100 1.98791000
H 0.08288400 -2.21596600 0.94978600
H 0.67649500 -0.06489400 1.84166500
H 2.38540400 -0.87533400 -1.64412900

21
E = -422.702342 a.u.

C -0.64929900 -0.03725300 -0.23733300
C -1.33014900 -1.15549900 0.03124400
C 1.44360000 1.21890900 0.02758800
C 2.82523500 0.63116300 0.31535300
C 2.47920300 -0.84633400 0.51143100
N 0.69333100 0.10072300 -0.58935800
H 1.48165300 2.08061600 -0.64276200
H 3.48787200 0.74965600 -0.54703500
H 2.05454300 -1.01440900 1.50621200
C -1.55742300 1.17014500 -0.29990700
C -2.84241700 0.65757300 0.37220100
H -1.14993600 2.05521000 0.19699400
C -2.80131600 -0.87378400 0.19382200
H -0.89080100 -2.14267700 0.04100500
H -3.74561700 1.11510600 -0.03675500
H -3.36283100 -1.18418600 -0.69842100
H 0.96714000 1.53113200 0.96440900
H 3.30071600 1.09358500 1.18179300
H 3.32181900 -1.52621700 0.37529500
H -1.72072500 1.44344700 -1.35030800
H -2.80526200 0.89450500 1.43935300
H -3.25073500 -1.39808600 1.04284500
N 1.45063300 -1.10883400 -0.49140700
H 1.89981500 -1.23042200 -1.39365200

TS-21-o
E = -818.463156 a.u.
Freq = 457.96i cm^{-1}

N 0.81424000 -0.94978700 0.74918400
N 0.08672500 -0.34351700 1.60028400
N -1.05263100 -0.13398100 1.71089600
C -1.75973700 -0.56819400 -0.36983700
C -0.65178100 -1.29852700 -0.77945400
C -3.01210900 1.52971300 -0.03354000
C -2.42656500 2.94426800 -0.05132200
C -0.93303000 2.65487200 -0.21899300
N -2.04440300 0.72514000 -0.80689200
H -4.00322200 1.48218200 -0.49093700
H -2.79893100 3.51059000 -0.91011400
H -0.48578000 2.37846300 0.73910600
C -2.88978300 -1.49865900 0.01703200
C -2.14779400 -2.80881900 0.31372000
H -3.48559800 -1.14491200 0.86047200
C -0.93865600 -2.77224500 -0.63646300
H 0.04757700 -0.91038900 -1.50605700
H -2.77425700 -3.69164000 0.17536100
H -1.21505800 -3.18070700 -1.61850200
H -3.07861400 1.15571200 0.99131500
H -2.66403000 3.50045600 0.85666700

H -0.36134500 3.48196800 -0.64299000
H -3.56277400 -1.61070800 -0.84368500
H -1.80002000 -2.80204600 1.35038300
H -0.08886100 -3.34953100 -0.26718700
N -0.88633500 1.50238000 -1.11870400
H -1.01173700 1.83115800 -2.07097400
C 2.06379200 -0.40184200 0.41866700
C 2.84746600 -1.13739200 -0.47205100
C 2.52452900 0.83224100 0.88347700
C 4.06811700 -0.63838200 -0.90013700
H 2.48438400 -2.09787900 -0.81898800
C 3.75556300 1.31307400 0.46213600
H 1.92071400 1.40137000 1.58054100
C 4.53153800 0.58692500 -0.43404100
H 4.66629600 -1.21635100 -1.59559300
H 4.10862800 2.26800600 0.83540400
H 5.49015600 0.97041800 -0.76277300

TS-21-m
E = -818.478352 a.u.
Freq = 328.74i cm^{-1}

N -1.24411100 -1.15419400 -1.90106400
N -0.19055800 -1.17432500 -1.38602500
N 0.26166200 -0.87726300 -0.22370800
C -2.03221900 0.21327400 0.36271400
C -2.67126300 -0.40006600 -0.71114700
C -0.43330600 1.83687400 1.28101000
C 0.46855200 2.72541500 0.41229300
C -0.03887100 2.43706200 -1.00623700
N -1.56087900 1.48176800 0.39811700
H -0.78793200 2.34600200 2.17970200
H 0.33312800 3.78161700 0.65970900
H 0.44755300 1.55214100 -1.41935000
C -2.16943000 -0.61234800 1.61693500
C -2.60709800 -1.97931700 1.07525500
H -1.26798300 -0.65362800 2.22733500
C -3.38367300 -1.63692300 -0.20715700
H -3.05304600 0.19143300 -1.52955400
H -3.19484700 -2.54953200 1.79643400
H -4.43235600 -1.40745500 0.02428900
H 0.08782100 0.92270600 1.56634500
H 1.52134200 2.47030700 0.54024500
H 0.09985000 3.26662900 -1.70055600
H -2.96504300 -0.15880600 2.22460900
H -1.71611100 -2.55867900 0.82119000
H -3.37869500 -2.45070100 -0.93541600
C 2.17871700 -0.78426500 1.19577700
C 3.54020000 -0.62720600 1.40588700
C 4.41057500 -0.49249100 0.32930100
C 3.89670600 -0.51923300 -0.96212200
C 2.53426400 -0.66392700 -1.18264800
C 1.65439700 -0.80014100 -0.10164000
H 1.50164700 -0.91389400 2.03324700

H 3.92576700 -0.62043800 2.41961300
H 5.47474400 -0.37338800 0.49468400
H 4.56316900 -0.41919000 -1.81206600
H 2.13973800 -0.67854100 -2.19233100
N -1.46846100 2.15796900 -0.84654500
H -1.96761400 3.03549100 -0.73288700

CA-21-o
E = -818.548706 a.u.

N 0.80018300 0.18269100 -0.34607500
N 0.11672200 -0.29996700 -1.41164500
N -1.09334500 -0.03297400 -1.36785400
C -1.43660200 0.67249700 -0.09775800
C -0.07077800 0.85240400 0.60628900
C -3.69914600 -0.28956400 0.00710400
C -3.97467700 -1.79354100 0.10705100
C -2.55823500 -2.35941200 0.22160000
N -2.38875600 -0.08846200 0.68329300
H -4.47037300 0.30828800 0.49744300
H -4.54755900 -2.02544900 1.00999700
H -2.08329600 -2.41653600 -0.76010900
C -1.94060400 2.08814100 -0.41180700
C -0.66618300 2.93333300 -0.46401100
H -2.51853700 2.11419200 -1.33666500
C 0.17247400 2.36637100 0.68502900
H -0.03877000 0.34162000 1.56881500
H -0.86125200 4.00256400 -0.36570500
H -0.20692400 2.73450600 1.64390300
H -3.63616500 0.01021300 -1.04205900
H -4.52669400 -2.17029400 -0.75547900
H -2.50713500 -3.34051300 0.69737300
H -2.58288900 2.41461100 0.41201000
H -0.15033800 2.77557200 -1.41662600
H 1.23200100 2.62109700 0.62149200
N -1.84711100 -1.37016000 1.03439700
H -2.09396800 -1.51465800 2.00755500
C 2.13519700 -0.16979700 -0.14213800
C 2.77110200 0.17310200 1.05333600
C 2.85341400 -0.85439000 -1.12916800
C 4.10356500 -0.16568600 1.25439700
H 2.23180300 0.70209600 1.82887300
C 4.18002700 -1.18494300 -0.91024900
H 2.35814700 -1.12267300 -2.05194600
C 4.81818100 -0.84455200 0.27883100
H 4.58143400 0.10719600 2.18866700
H 4.72317700 -1.71731200 -1.68316200
H 5.85707100 -1.10619400 0.43977600

CA-21-m
E= -818.540400 a.u.

N -1.93391300 -1.17087300 -1.71079000

N -0.79437200 -1.52894600 -1.39006200
N -0.34246800 -0.92874500 -0.24530600
C -1.25853200 0.16265900 0.18512700
C -2.43965900 -0.16458700 -0.77296800
C 0.04251500 2.13005600 1.07543300
C 1.00771600 3.03708800 0.31344500
C 1.16213600 2.27258600 -1.00198200
N -0.77788900 1.51116400 0.01558200
H -0.59030600 2.69000100 1.76884600
H 0.55628400 4.01730900 0.13348600
H 1.87308600 1.45143700 -0.88655800
C -1.82592200 -0.07513700 1.59532500
C -2.87122900 -1.16930700 1.38896800
H -1.06347000 -0.32879800 2.33139300
C -3.57301400 -0.72502700 0.10136500
H -2.75055400 0.70704100 -1.34903000
H -3.55282100 -1.26830000 2.23576700
H -4.29006100 0.07064400 0.32472800
H 0.60309000 1.38542100 1.64723700
H 1.94850100 3.18091800 0.84683400
H 1.48368900 2.89212200 -1.84101100
H -2.31477900 0.84742300 1.92402500
H -2.37700100 -2.13382800 1.23862800
H -4.10668100 -1.52658400 -0.41079500
C 1.56129000 -0.96714400 1.27725400
C 2.93274600 -1.01318300 1.48992000
C 3.80764200 -1.14090800 0.41904400
C 3.29418400 -1.22217900 -0.87051200
C 1.92759800 -1.14528600 -1.09382500
C 1.04740600 -1.00887400 -0.01813500
H 0.89012600 -0.91418300 2.12433200
H 3.31533500 -0.97032300 2.50350800
H 4.87701700 -1.18766300 0.58788600
H 3.96438400 -1.32905200 -1.71611300
H 1.52421600 -1.17901000 -2.09665300
N -0.17377300 1.73278500 -1.26760800
H -0.72241500 2.46317500 -1.70997400

22
E = -289.967291 a.u.

C 1.67434300 0.55167200 -0.00990800
C 2.69750800 -0.31392300 0.03334700
C -0.71146700 1.22507400 -0.16393100
C -1.96113700 0.46063000 0.26719200
C -1.65348500 -0.96863000 -0.19435800
C -0.14595300 -1.11433300 0.05147800
N 0.34391300 0.25018400 0.04304900
H -0.53667600 2.12331800 0.43527100
H -2.05566400 0.49408100 1.35646800
H -1.86653500 -1.06503900 -1.26301900
H 0.34256000 -1.71370400 -0.72792500
H 2.55319300 -1.38453600 0.11148500
H -0.78864100 1.53103900 -1.21908300

H -2.87604200 0.86476300 -0.16897100
H -2.23836600 -1.72450700 0.33146700
H 0.07314800 -1.59395500 1.01536800
H 1.87402200 1.61813200 -0.07968000
H 3.71275500 0.05618200 0.00435500

TS-22-o
E = -685.721048 a.u.
Freq = 482.25i cm^{-1}

N -1.06567600 -1.45671200 1.55585100
N 0.08314400 -1.30452800 1.41715300
N 0.87814700 -1.43753500 0.41927200
C -1.72389800 -1.44929800 -0.56040000
C -0.48380400 -1.73691600 -1.11805400
C -3.56537800 0.02614900 0.08728500
C -3.77159600 1.52920900 -0.06810400
C -2.33812100 2.06403800 -0.00354200
C -1.52731900 1.00564600 -0.75940300
N -2.32310800 -0.21408100 -0.63750100
H -4.38251100 -0.56094500 -0.34210400
H -4.21522600 1.74790300 -1.04402200
H -2.00842700 2.10414500 1.03874800
H -0.52779700 0.87799700 -0.32880200
H 0.00276200 -1.02155100 -1.77033200
H -3.46379700 -0.24873500 1.14655200
H -4.42079700 1.94482700 0.70382800
H -2.22757200 3.06164700 -0.43099300
H -1.39625600 1.27530800 -1.81471400
C 2.78627100 -0.71169800 -0.81125800
C 3.79913900 0.19781900 -1.07300600
C 3.97466200 1.31240300 -0.26009100
C 3.12028700 1.51013900 0.81779100
C 2.09130000 0.61632800 1.08031400
C 1.91903000 -0.50520800 0.26396200
H 2.65542200 -1.59199900 -1.42959800
H 4.46351000 0.02816900 -1.91278600
H 4.77323100 2.01644700 -0.46130800
H 3.25089600 2.37179000 1.46292500
H 1.42876300 0.77235300 1.92340600
H -2.39778000 -2.26409300 -0.32668900
H -0.22540800 -2.77493000 -1.27051000

TS-22-m
E = -685.737424 a.u.
Freq = 353.17i cm^{-1}

N -0.81884900 2.63171200 0.55473800
N 0.13479700 1.95382900 0.41942700
N 0.45179300 0.98758100 -0.35198600
C -1.94333000 0.80090200 -1.16279900
C -2.21179100 2.10700100 -0.76921400
C -1.72203100 -1.59484700 -0.80984000

C -2.30260800 -2.51761700 0.25561000
C -2.38639500 -1.59723800 1.47698600
C -2.81130800 -0.25073900 0.88399800
N -2.30810400 -0.29584400 -0.48990500
H -1.97529500 -1.89452800 -1.82917700
H -3.30115700 -2.85425900 -0.03874000
H -1.39767200 -1.50089600 1.93360000
H -2.37467000 0.59678900 1.41874800
H -3.02205900 2.29526700 -0.07681500
H -0.62864400 -1.52491700 -0.72251500
H -1.68086600 -3.39720900 0.42435900
H -3.07959300 -1.95300000 2.23987900
H -3.90046500 -0.12968300 0.88183200
C 2.09602100 -0.57781000 -1.07462800
C 3.31226000 -1.23092300 -0.94349100
C 4.17124000 -0.91973000 0.10446300
C 3.79430200 0.05777100 1.01865300
C 2.57850200 0.71491200 0.89840400
C 1.71023300 0.40172500 -0.15388200
H 1.43045000 -0.80725700 -1.89952800
H 3.59285800 -1.98576200 -1.67001000
H 5.12201500 -1.42940700 0.20606700
H 4.45445500 0.31346100 1.84051100
H 2.29017800 1.47387000 1.61593700
H -1.42636400 0.61268600 -2.09476500
H -2.03119800 2.88345800 -1.50085600

CA-22-o
E= -685.796945 a.u.

N -1.02157600 -1.64787800 0.44739800
N 0.14034500 -1.34049300 0.75096100
N 0.73492200 -0.54347600 -0.17638300
C -1.43154600 -0.94779800 -0.81545400
C -0.11551300 -0.35004100 -1.33333800
C -3.78357800 -0.49869300 -0.29513600
C -4.53479400 0.74182400 0.16521200
C -3.49465900 1.43478700 1.05385500
C -2.14353000 1.09302000 0.39864600
N -2.44907800 0.02881100 -0.57247200
H -4.20414300 -0.94909900 -1.19915200
H -4.78008000 1.36527300 -0.69905500
H -3.53368900 1.01231700 2.06106200
H -1.42147500 0.76982100 1.15811800
H -0.22505900 0.70569700 -1.58682700
H -3.77500500 -1.26096300 0.49867000
H -5.45921300 0.50686800 0.69520900
H -3.65646800 2.51026700 1.13978700
H -1.71385800 1.95601900 -0.12056700
C 2.67954100 0.56724000 -1.07297800
C 4.00154900 0.97508400 -0.94277500
C 4.72435600 0.67995700 0.20336100
C 4.10674000 -0.03249200 1.22728400
C 2.78959300 -0.44492400 1.11729100

C 2.06486500 -0.14566200 -0.04170300
H 2.13172300 0.80501100 -1.97658200
H 4.46520400 1.52814000 -1.75186400
H 5.75499200 0.99910300 0.30051900
H 4.65845700 -0.27163100 2.12953100
H 2.31050900 -0.99864700 1.91286100
H -1.83818600 -1.70006500 -1.49287200
H 0.27585600 -0.89067200 -2.20095300

CA-22-m
E= -685.798367 a.u.

N 1.33434200 -2.69853100 0.43768000
N 0.18512000 -2.25628200 0.59540600
N -0.13596000 -1.29651500 -0.32248500
C 1.09958500 -0.79520600 -0.97655800
C 1.95756500 -2.03568600 -0.72024900
C 1.20720700 1.70473700 -0.86313200
C 2.12639600 2.62811400 -0.07164400
C 2.22033400 1.93092600 1.29999600
C 1.85275200 0.45637400 1.02545100
N 1.66454200 0.39318600 -0.42150600
H 1.31922000 1.80215300 -1.94675200
H 3.10758000 2.66094800 -0.55091100
H 1.51019500 2.36826800 2.00458900
H 0.93398600 0.18513400 1.56745100
H 2.99923300 -1.79298500 -0.51423500
H 0.15637000 1.90373700 -0.60455800
H 1.74325900 3.64747800 -0.00243100
H 3.21499600 2.02977500 1.73664000
H 2.63012400 -0.24540500 1.34025300
C -1.80850600 0.21025000 -1.20044300
C -2.97172300 0.94985400 -1.04572900
C -3.67444000 0.91616000 0.15254400
C -3.19731700 0.13304700 1.19652300
C -2.02468900 -0.59661900 1.06093900
C -1.32042600 -0.55888500 -0.14332100
H -1.27707100 0.22903500 -2.14469500
H -3.33555400 1.54764500 -1.87376500
H -4.58619500 1.48968600 0.26927700
H -3.73740900 0.09420400 2.13584900
H -1.65006400 -1.20433600 1.87346300
H 0.92038900 -0.63269800 -2.03887800
H 1.91419600 -2.73403700 -1.56123600

23
E = -481.895395 a.u.

C -1.13546300 1.23963500 0.13191300
C -2.59453100 0.99130000 0.47073400
C -2.29245400 -1.07101000 -0.68282300
C -1.13313300 -1.21020800 0.29420400
N -0.36832700 0.02781300 0.34709800

H -1.04815800 1.58401300 -0.91155300
H -2.68224700 0.73249800 1.53545600
H -2.87951700 -1.99277400 -0.70558500
H -1.52105100 -1.47479100 1.28656400
C 0.98281600 0.06926800 0.08475000
C 1.71607600 1.14004400 -0.26606300
C 1.84270800 -1.17107900 0.19203700
C 3.17033700 0.78342800 -0.43950400
H 1.32816200 2.13185600 -0.45623400
C 3.26818900 -0.59669100 0.24066800
H 1.69877500 -1.80961400 -0.68954300
H 1.60355000 -1.77595900 1.07164500
H 3.44303700 0.72381200 -1.50229500
H 3.85123500 1.50907400 0.01635400
H 4.00392700 -1.25535700 -0.22543500
H 3.55967000 -0.46107200 1.28574600
H -0.49620200 -2.03190000 -0.03343400
H -1.89160700 -0.89425600 -1.69062600
H -3.17438100 1.89930500 0.29763300
H -0.74302800 2.03944000 0.77101300
O -3.17764400 -0.02088600 -0.32936200

TS-23-o
E = -877.654177 a.u.
Freq =459.8i cm^{-1}

C 0.89340300 -1.35397800 -0.91879700
C 1.03034500 -2.51176400 0.05899700
C 3.34663800 -2.25466200 -0.39688400
C 3.09408700 -0.81682700 0.02085300
N 1.89360900 -0.32181900 -0.64650800
H 0.99673400 -1.72352000 -1.94581700
H 0.84426000 -2.14463200 1.07754400
H 4.26068200 -2.62002200 0.07506900
H 2.99788000 -0.75959800 1.11408100
C 1.47252900 0.95994000 -0.34145900
C 0.28752300 1.54277000 -0.79402000
C 2.47904800 2.04003800 0.00360000
C 0.40538200 3.04483400 -0.73066400
H -0.34767000 1.07418800 -1.53471700
C 1.59210500 3.27174200 0.21939300
H 3.14881100 2.18192600 -0.85567200
H 3.09472200 1.80247000 0.87230300
H 0.64183700 3.42868900 -1.73253000
H -0.50991200 3.53718500 -0.39672700
H 2.11682200 4.20936100 0.02936800
H 1.23878200 3.28767700 1.25375300
H 3.95588800 -0.21049100 -0.27185100
H 3.48675100 -2.29385400 -1.48654100
H 0.28831900 -3.28049200 -0.16774400
H -0.11245400 -0.94318300 -0.82242500
O 2.30353700 -3.13004000 -0.00924100
N 0.79705500 0.63130300 1.76234400
N -0.36127100 0.66039000 1.63904800

N -1.14479900 1.09203500 0.72020400
C -2.27178300 0.31715500 0.39890800
C -2.52717500 -0.95006800 0.93219300
C -3.13201100 0.84159100 -0.56846000
C -3.63126200 -1.67168000 0.50053000
H -1.86816300 -1.35543800 1.69139800
C -4.22180000 0.10329800 -1.00385700
H -2.93220500 1.82971100 -0.96656500
C -4.47993800 -1.15527700 -0.47152000
H -3.82599400 -2.64908900 0.92755200
H -4.88047800 0.51922200 -1.75784900
H -5.33761300 -1.72582300 -0.80718300

TS-23-m
E = -877.670509 a.u.
Freq = 345.27i cm^{-1}

C -1.85226000 1.46239900 -1.18530900
C -0.66724800 2.40812800 -1.31521200
C -1.31444700 3.14788800 0.84419700
C -1.19150600 1.67075900 1.17390500
N -1.87533900 0.87960500 0.15853600
H -2.78925000 1.99368000 -1.38466100
H 0.26104600 1.83908600 -1.17468600
H -0.80713900 3.73431000 1.61295800
H -0.13349700 1.37289600 1.21803500
C -1.96671500 -0.45261900 0.31420300
C -2.36485500 -1.37903700 -0.65142500
C -1.81588300 -1.11880200 1.66075900
C -2.62430500 -2.70834400 0.02250000
H -2.95079800 -1.07989800 -1.50988700
C -1.78584500 -2.61074000 1.30661100
H -2.70571400 -0.87459700 2.25858500
H -0.93724500 -0.79296900 2.21567800
H -3.69048300 -2.81712400 0.26156500
H -2.34031900 -3.55652200 -0.60426200
H -2.15992200 -3.24203100 2.11406400
H -0.75380900 -2.89921200 1.09396400
H -1.64096200 1.48734300 2.15201700
H -2.37693200 3.42978700 0.84748000
H -0.65368300 2.84472700 -2.31508700
H -1.74362700 0.66723800 -1.92359100
O -0.73079600 3.48576400 -0.39888900
C 1.95028200 -0.58271300 -0.07375500
C 2.91846800 -0.71840600 -1.07488300
C 4.24519700 -0.41333700 -0.80811500
C 4.63520800 0.03472900 0.44897200
C 3.67577900 0.17020700 1.44568800
C 2.34770600 -0.13623700 1.19005400
H 2.62104600 -1.06325900 -2.05822300
H 4.98247200 -0.52412000 -1.59588600
H 5.67281200 0.27426200 0.64885700
H 3.96342500 0.51331200 2.43345600
H 1.60023700 -0.04605300 1.97070400

N 0.58066000 -0.83782300 -0.24695000
N 0.24338700 -1.40367200 -1.34051600
N -0.76424300 -1.75099700 -1.83665800

CA-23-o
E = -877.735299 a.u.

C -1.82117300 -1.28778700 0.80278800
C -2.61151000 -2.23704700 -0.08626900
C -4.40744700 -0.79483500 0.48520200
C -3.47859900 0.27443300 -0.06019700
N -2.14714300 0.12573800 0.54032500
H -2.03396400 -1.51784000 1.85262900
H -2.35484500 -2.04932400 -1.13646500
H -5.41465800 -0.64387700 0.09144600
H -3.44575300 0.19311600 -1.15619500
C -1.11864500 0.87266700 -0.13741700
C 0.24162800 0.91449000 0.61325600
C -1.49117600 2.34085900 -0.38692300
C 0.62085800 2.39835900 0.73264500
H 0.20255800 0.40343900 1.57723000
C -0.14648200 3.06657200 -0.41103600
H -2.09145500 2.69364100 0.45768100
H -2.07112100 2.45757800 -1.30316800
H 0.26394900 2.77795600 1.69546800
H 1.70043600 2.55271800 0.68865800
H -0.24466900 4.14609700 -0.28648700
H 0.36294100 2.88634600 -1.36297400
H -3.88709900 1.25721500 0.19060600
H -4.45410100 -0.70894000 1.58049500
H -2.35790100 -3.27287300 0.15034100
H -0.75625300 -1.47149800 0.64515700
O -4.00949600 -2.10158100 0.11339600
N -0.77276400 0.22727900 -1.44707400
N 0.40780100 -0.14949300 -1.45897900
N 1.07803000 0.18386100 -0.32379400
C 2.38782300 -0.25317000 -0.11264500
C 3.08542700 -0.93404100 -1.11650600
C 3.01260400 -0.00884100 1.11253700
C 4.38268900 -1.35910400 -0.88396300
H 2.59939200 -1.12358900 -2.06344900
C 4.31521900 -0.44254400 1.32676700
H 2.48914400 0.51853400 1.90019200
C 5.00973600 -1.11858200 0.33490200
H 4.91123700 -1.88658900 -1.67008200
H 4.78556300 -0.24558900 2.28354200
H 6.02539400 -1.45413900 0.50601700

CA-23-m
E = -877.730778 a.u.

C 0.01383500 1.55830700 -1.30785500
C 1.46374100 2.00288800 -1.18000900
C 0.69117500 3.26315000 0.67852100
C 0.17528800 1.90174300 1.11332700

N -0.58155100 1.31879500 0.01128100
H -0.55347600 2.32579700 -1.84912700
H 2.05965300 1.19062400 -0.74251600
H 1.22071400 3.74132800 1.50625900
H 1.02344700 1.28417600 1.43895200
C -1.28469600 0.08356100 0.18836700
C -2.47766300 -0.09945000 -0.80037500
C -1.91855500 -0.07993900 1.58102800
C -3.69475000 -0.49731700 0.04932600
H -2.66544900 0.79414300 -1.39722500
C -3.08434400 -1.03666600 1.34555200
H -2.30929900 0.89348900 1.89346200
H -1.21604500 -0.42003300 2.34123000
H -4.29625500 0.39118100 0.26314200
H -4.32537100 -1.21372600 -0.47828500
H -3.79073000 -1.05270700 2.17731700
H -2.71251100 -2.05497800 1.19832200
H -0.47870000 2.04500400 1.97686000
H -0.16466700 3.89545600 0.40424700
H 1.87214400 2.22682100 -2.16723300
H -0.01067700 0.64881400 -1.91480000
O 1.59512200 3.18410700 -0.41046700
C 0.86090400 -1.35712100 0.03259400
C 1.72375100 -1.66594200 -1.02139000
C 3.07657900 -1.85749200 -0.78121800
C 3.59428500 -1.72315100 0.50121500
C 2.73562700 -1.42250500 1.55058200
C 1.37636200 -1.25632100 1.32389700
H 1.32222400 -1.76101900 -2.02157100
H 3.73276900 -2.09902600 -1.60967500
H 4.65378800 -1.85932100 0.68219700
H 3.12086100 -1.33052200 2.55972500
H 0.71648100 -1.05304000 2.15634800
N -0.51542000 -1.14360800 -0.20670000
N -1.02216700 -1.69796600 -1.34787900
N -2.09073600 -1.18404900 -1.71031400

24
E=-212.547628 a.u.

C 0.79500200 -0.66535300 0.11899600
C 1.99033400 -0.11381400 -0.11796500
C -1.60286400 -0.75339600 -0.13737600
C -0.45390100 1.39910800 0.00251900
N -0.41875000 -0.02045300 0.26086400
H -1.52059800 -1.79136200 0.19178100
H 0.27778300 1.91022000 0.63295600
H 2.13132700 0.94735600 -0.27936000
H -2.48533400 -0.31845200 0.33883400
H -0.23154000 1.64283300 -1.04918800
H 2.87083300 -0.74158500 -0.13366800
H -1.44433600 1.78636300 0.24853200
H -1.76062600 -0.74979400 -1.22731900
H 0.72232300 -1.74167200 0.25433800

TS-24-o
E = -608.300295 a.u.
Freq = 482.48i cm^{-1}

N -1.72456300 -0.69972000 1.60252700
N -0.56906900 -0.79717800 1.47921700
N 0.19421600 -1.17436600 0.52354300
C -2.34665900 -0.76194600 -0.52356400
C -1.19877400 -1.36743400 -1.01170600
C -3.82066300 1.05682700 0.01831300
C -1.61333400 1.52463600 -0.87834500
N -2.69092800 0.56553100 -0.74851000
H -4.62273300 0.31644200 0.00684000
H -1.05641800 1.66113100 0.06294600
H -0.54916800 -0.86443200 -1.71615000
H -3.55941000 1.26672900 1.06491200
H -0.90647600 1.21960600 -1.65072700
C 2.21740800 -0.96440200 -0.71804700
C 3.39707300 -0.30726800 -1.03237200
C 3.79150700 0.81661300 -0.31486800
C 2.98885400 1.27978700 0.72077900
C 1.79685500 0.64170600 1.03383500
C 1.40382500 -0.48901600 0.31274300
H 1.91393800 -1.85253500 -1.25987700
H 4.01833200 -0.68361900 -1.83719500
H 4.71855800 1.32262900 -0.55646200
H 3.28918000 2.15101600 1.29206800
H 1.17536900 1.00410300 1.84394400
H -1.17746900 -2.44766600 -1.03914200
H -2.02893100 2.48914300 -1.17565000
H -4.20108500 1.97240100 -0.44081700
H -3.17783100 -1.39184500 -0.2327420

TS-24-m
E = -608.315413 a.u.
Freq = 356.37i cm^{-1}

N 1.51478300 -2.23761000 0.00023100
N 0.46504500 -1.70339800 0.01135800
N 0.03816700 -0.56780100 -0.38381600
C 2.36409400 0.23863600 -0.85722900
C 2.84489800 -1.06589300 -0.86870700
C 1.60231600 2.25996400 0.16638900
C 2.91336000 0.64119500 1.45770100
N 2.49982300 1.12100700 0.15317600
H 1.45059000 2.62140800 -0.85119300
H 2.15764400 -0.02968800 1.88779400
H 3.62069000 -1.36036000 -0.17491400
H 0.62680400 1.97773700 0.58510000
H 3.86080800 0.10524400 1.38929000
C -1.79829300 0.91664400 -0.70721600
C -3.12384400 1.28624600 -0.53528600
C -4.00045200 0.46532000 0.16479400
C -3.52988400 -0.73355400 0.68883100

C -2.20547600 -1.11172900 0.52459900
C -1.31989400 -0.28546400 -0.17689700
H -1.11565100 1.54845600 -1.26423300
H -3.47504500 2.22197200 -0.95644600
H -5.03624400 0.75406600 0.29814200
H -4.20196300 -1.38596500 1.23583000
H -1.84498000 -2.04649200 0.93703400
H 2.87427700 -1.55786100 -1.83221400
H 3.05372400 1.49350600 2.12233000
H 2.03497100 3.06811900 0.75862400
H 1.88868900 0.63628900 -1.74366100

CA-24-o
E= -608.378731 a.u.

N 1.71598400 1.24228400 -0.69428400
N 0.51260500 1.34098700 -0.41361600
N -0.11362400 0.13589100 -0.34341700
C 2.11491800 -0.19980600 -0.77195600
C 0.77263000 -0.94237400 -0.73087000
C 4.36461100 -0.05252100 0.08436800
C 2.52562900 -0.25966800 1.62523800
N 3.01888700 -0.56737600 0.28972400
H 4.73286100 -0.36569300 -0.89579100
H 2.47157000 0.82096100 1.82514500
H 0.78148600 -1.75283200 0.00022600
H 4.42000900 1.04453600 0.14341700
H 1.52912800 -0.68155900 1.77339500
C -2.12174300 -1.19392200 -0.20430000
C -3.48987600 -1.29106500 0.01913600
C -4.24065700 -0.16376800 0.31676400
C -3.60473700 1.07220400 0.39038100
C -2.24217800 1.18869000 0.17364900
C -1.48953300 0.04852300 -0.12812700
H -1.55203200 -2.08524200 -0.43705600
H -3.96705500 -2.26256900 -0.04331900
H -5.30706000 -0.24372500 0.48967800
H -4.17789700 1.96297300 0.62191000
H -1.74857300 2.14892800 0.23099400
H 0.49290900 -1.34586400 -1.70920400
H 3.19036900 -0.71632400 2.36157500
H 5.02772600 -0.47505800 0.84310000
H 2.63521300 -0.34879600 -1.71862800

CA-24-m
E = -608.379967 a.u.

N 2.27301700 -1.86223100 -0.09201800
N 1.03752100 -1.83692700 0.02521700
N 0.48637200 -0.69919000 -0.48895800
C 1.53529900 0.32402200 -0.71733900
C 2.72522000 -0.63814300 -0.77410400
C 0.82386300 2.51019500 0.16020600
C 1.72337700 0.84277600 1.65825100
N 1.66978200 1.33652800 0.29374000

H 0.79061000 2.82516800 -0.88562500
H 0.75760100 0.44147400 2.00574800
H 3.61572600 -0.23319700 -0.29404800
H -0.20761100 2.35309700 0.50751600
H 2.47140100 0.05333500 1.75481900
C -1.53104900 0.51000400 -1.04856100
C -2.87675900 0.77727600 -0.84314900
C -3.59435300 0.08203700 0.12217100
C -2.94796100 -0.88508100 0.88253000
C -1.59789100 -1.14819700 0.70035100
C -0.87967000 -0.44662200 -0.26941900
H -0.98522300 1.04337800 -1.81761700
H -3.36856500 1.52732000 -1.45219000
H -4.64671300 0.28820600 0.27666100
H -3.49651300 -1.43793300 1.63677500
H -1.09166100 -1.89789700 1.29331300
H 2.97321300 -0.90876500 -1.80423000
H 2.01100600 1.66087300 2.32223300
H 1.25856500 3.32987800 0.73957300
H 1.37086800 0.81820300 -1.67441200

26
E = -193.096927 a.u.

C -0.60950400 0.34896800 -0.03107800
C -1.86592400 -0.07110400 0.03346300
C 1.71316400 0.10901100 0.03906900
H 1.87149400 0.83351500 -0.76881500
H -2.09988800 -1.12725400 0.08269500
H 1.84308100 0.60972500 1.00545100
H -2.67399500 0.64678400 0.02975400
H 2.45003700 -0.68753300 -0.05048200
H -0.35825900 1.40829000 -0.08023500
O 0.44263900 -0.50059700 -0.05838600

TS-26-o
E = -588.850947 a.u.
Freq = 493.62 i cm^{-1}

N 1.87858700 -0.86917900 1.25081000
N 0.73011800 -0.67515900 1.25773500
N -0.02063300 0.29921200 0.94707900
C 2.55102600 0.77570900 0.03145700
C 1.41613400 1.55553800 0.03988800
C 4.01095300 -0.71865400 -1.00961500
H 4.89860500 -0.13011500 -0.74450300
H 0.84162900 1.66161500 -0.87195000
H 3.86362400 -1.50698800 -0.26600700
C -2.08727700 1.17952600 0.15276100
C -3.34230100 1.02827600 -0.41711100
C -3.83046100 -0.23751200 -0.72067300
C -3.04611000 -1.35368300 -0.45440500
C -1.78186900 -1.21476100 0.09969600
C -1.29767500 0.05794800 0.40860200
H -1.70633200 2.16140500 0.40789600

H -3.94650000 1.90601600 -0.61625000
H -4.81493100 -0.35350600 -1.15794800
H -3.41778900 -2.34575400 -0.68468200
H -1.16996600 -2.08570200 0.30233100
H 1.31733600 2.32634400 0.78986000
H 4.16044800 -1.16395100 -1.99194500
H 3.36454800 0.96419400 0.72695500
O 2.86728600 0.10599900 -1.10834000

TS-26-m
E = -588.859284 a.u.
Freq = 395.68i cm^{-1}

N -1.93182100 -2.11869500 -0.10227600
N -0.84802000 -1.67109200 -0.05285100
N -0.38122900 -0.53819600 0.28950700
C -2.47569600 0.49480900 0.45807800
C -3.16646000 -0.69937200 0.50351200
C -1.58231900 2.28786900 -0.73417500
H -1.59931700 2.90159200 0.17327600
H -3.88435700 -0.89141800 -0.28311500
H -0.57908300 1.87966400 -0.88358800
C 1.48865000 0.87733800 0.72834300
C 2.83469400 1.19583000 0.62576600
C 3.71347800 0.34255100 -0.03093800
C 3.22624500 -0.83624400 -0.58422600
C 1.88105300 -1.16209800 -0.49422400
C 0.99613500 -0.30334400 0.16578100
H 0.80521400 1.53306000 1.25602400
H 3.19965600 2.11537000 1.06971600
H 4.76519600 0.59092100 -0.10801400
H 3.90048600 -1.51267300 -1.09789900
H 1.50536900 -2.07962400 -0.93085100
H -3.37349500 -1.12091700 1.47809700
H -1.87146800 2.89533800 -1.58911800
H -2.05029800 0.95731200 1.34197200
O -2.52313600 1.23040100 -0.64933400

CA-26-o
E = -588.932933 a.u.

N -1.99308600 1.18288900 0.43913600
N -0.76835100 1.30046100 0.26729400
N -0.11969200 0.11729300 0.25816000
C -2.36342200 -0.25472700 0.50468700
C -1.02766000 -0.99282700 0.47651400
C -4.40739000 -0.04256200 -0.63426000
H -4.98020300 -0.32864100 0.25857400
H -1.00906200 -1.70427900 -0.35156100
H -4.35507900 1.04785400 -0.69146300
C 1.89115900 -1.20321100 0.08282000
C 3.26678300 -1.28685100 -0.09461900
C 4.02751000 -0.14212600 -0.27908100
C 3.39463700 1.09741700 -0.28546800

C 2.02489600 1.20091400 -0.11091400
C 1.26312300 0.04305000 0.07586800
H 1.31290700 -2.10821000 0.22334100
H 3.74152000 -2.26144400 -0.08784700
H 5.09967200 -0.21162200 -0.41730100
H 3.97563200 2.00137300 -0.42950600
H 1.53340700 2.16390900 -0.11698800
H -0.80173600 -1.50519700 1.41515300
H -4.90629600 -0.43367800 -1.51975100
H -2.93601700 -0.41481700 1.42724300
O -3.11558200 -0.62052700 -0.60941400

CA-26-m
E = -588.933345 a.u.

N -2.47397300 -1.67781100 -0.02450300
N -1.24100400 -1.69421100 -0.12196400
N -0.67260700 -0.51786300 0.29904000
C -1.68831500 0.51621900 0.43055800
C -2.91019400 -0.38400200 0.53057300
C -0.87096200 2.34230800 -0.86966200
H -0.71512600 2.89900200 0.06467000
H -3.74497400 0.01507700 -0.04308300
H 0.08953100 1.94269200 -1.20780300
C 1.35915200 0.62010300 0.96762800
C 2.73064700 0.80063700 0.86323500
C 3.48278700 0.00974000 0.00366700
C 2.84489000 -0.96442400 -0.75472700
C 1.47100900 -1.14176200 -0.67528500
C 0.71940100 -0.34505600 0.18867000
H 0.78646400 1.22851300 1.65753700
H 3.21421400 1.55810200 1.46962500
H 4.55470900 0.14817300 -0.07091300
H 3.41970400 -1.59051600 -1.42771800
H 0.97088800 -1.89464000 -1.26917000
H -3.22454000 -0.55462300 1.56355600
H -1.26279500 3.02259100 -1.62531600
H -1.50564700 1.12940800 1.31951900
O -1.83747900 1.32535700 -0.70085700

28
E = -272.711798 a.u.

C -1.27367800 -0.66639800 -0.50306600
C -0.08572100 -1.12257000 0.32361200
C -0.08505600 1.12292700 0.32279600
C -1.27328800 0.66659800 -0.50348400
H -1.91694200 -1.32140600 -1.07720300
H -1.91628700 1.32159900 -1.07792000
C -0.03636200 0.00059500 1.37605400
H 0.88505100 0.00057700 1.96657100
H -0.90419800 0.00113700 2.03818000
C 1.18228500 -0.77750300 -0.51748500
H 2.07836700 -1.17379400 -0.03287600
H 1.13056100 -1.20198300 -1.52151500

C 1.18297100 0.77642500 -0.51785000
H 2.07927300 1.17216000 -0.03310700
H 1.13173900 1.20058000 -1.52199200
H -0.11789900 -2.14832200 0.68903600
H -0.11656600 2.14900500 0.68736500

TS-28
E = -668.477259 a.u.
Freq = 403.79i cm^{-1}

C -2.24975000 0.86095300 -0.58344300
C -2.73087900 0.34606100 0.76307600
C -1.29314500 -1.19165800 -0.03703400
C -1.37809300 -0.09070200 -1.07383100
H -2.84754000 1.51044400 -1.21042700
H -1.17585100 -0.25631400 -2.12306100
C -1.47539300 -0.38877800 1.26117100
H -1.67369000 -1.02812700 2.12519500
H -0.63716400 0.26966600 1.49164200
C -3.65764800 -0.86282000 0.44883800
H -4.14257400 -1.21950400 1.36125800
H -4.44255500 -0.59994800 -0.26309300
C -2.66570500 -1.92394000 -0.11143400
H -2.64761900 -2.82025300 0.51369900
H -2.90837800 -2.23547800 -1.12953100
H -3.16301200 1.09418800 1.42603200
H -0.42236700 -1.84295900 -0.10164500
N 0.08538800 2.03890200 -0.31402900
N -0.94374400 2.50078800 -0.05009200
N 0.54242000 1.00578300 -0.88447900
C 1.71955200 0.41430300 -0.39676600
C 2.39827800 0.84854600 0.74387200
C 2.18245300 -0.70406500 -1.09196300
C 3.52846400 0.16749600 1.17388100
C 3.30416800 -1.38415500 -0.64402100
C 3.98502400 -0.95219700 0.48912500
H 2.04495500 1.72154300 1.28071600
H 4.05348000 0.51562900 2.05625700
H 4.86563800 -1.48139300 0.83300000
H 3.65349800 -2.25366300 -1.18915800
H 1.65078700 -1.02641600 -1.97950800

CA-28
E = -668.565801 a.u.

C -1.91416700 0.93517600 -0.70819900
C -2.93962600 0.50624400 0.35394500
C -1.36860000 -1.11577000 0.46491200
C -0.83637500 -0.17783200 -0.63801200
H -2.37007900 1.08570200 -1.68848800
H -0.64731300 -0.69435000 -1.58325900
C -2.03396400 -0.11896100 1.42640500
H -2.59882300 -0.61365700 2.21993400
H -1.33513900 0.58704500 1.87911600
C -3.67260900 -0.73197000 -0.19590800

H -4.52816100 -0.97794400 0.43659800
H -4.05084000 -0.57139400 -1.20835800
C -2.58662300 -1.84806200 -0.12797100
H -2.89823200 -2.66353000 0.52776400
H -2.36905300 -2.28380500 -1.10677700
H -3.58842300 1.32122500 0.67137000
H -0.60849700 -1.76859400 0.89307000
N -0.00543400 1.94129500 -0.11277000
N -1.20023500 2.17599300 -0.34364200
N 0.31254500 0.62548200 -0.25231900
C 1.63239600 0.19083700 -0.12145900
C 2.63998500 1.07296700 0.28491300
C 1.95681700 -1.13949100 -0.39809300
C 3.94253200 0.61907200 0.40698700
C 3.26934700 -1.57646100 -0.26910000
C 4.27058800 -0.70543500 0.13371200
H 2.38760400 2.10303400 0.49500300
H 4.71313100 1.31385900 0.72186600
H 5.29245700 -1.05067200 0.23410400
H 3.50408800 -2.61198700 -0.48856400
H 1.19093200 -1.83621300 -0.71505900

30
E= -195.312129 a.u.

C 0.27953600 -1.19662400 0.00000000
C -0.07199400 -0.32914400 1.22841000
C -0.07199400 1.07002400 0.66401000
C -0.07199400 1.07002400 -0.66401000
C -0.07199400 -0.32914400 -1.22841000
H -0.23496100 -2.15922500 0.00000000
H 0.63959400 -0.45846200 2.04885300
H -1.06324700 -0.57466400 1.63053300
H -0.11056200 1.95686900 1.28609500
H -0.11056200 1.95686900 -1.28609500
H 0.63959400 -0.45846200 -2.04885300
H -1.06324700 -0.57466400 -1.63053300
H 1.35403000 -1.39906900 0.00000000

TS-30
E = -591.074204 a.u.
Freq = 462.11i cm^{-1}

C 1.89040000 -1.08330900 1.35204700
C 1.31045900 -1.70414400 0.07049100
C 1.73773500 -0.72317700 -0.99526900
C 2.77930700 0.06210100 -0.54000000
C 3.14987700 -0.34087400 0.87277700
H 2.09666100 -1.82126900 2.12869900
H 0.23137000 -1.86921100 0.11750100
H 1.77749600 -2.67592900 -0.13791500
H 1.52542600 -0.88279800 -2.04333000
H 3.48751300 0.53634900 -1.20774100
H 3.41335600 0.50873600 1.50660000
H 4.01405700 -1.01706000 0.85061100

H 1.17265700 -0.36427000 1.76059400
C -1.18049800 0.43420500 -0.41816900
C -1.72400200 0.97927100 0.74774500
C -2.97152400 0.56103900 1.18778000
C -3.68068800 -0.40919300 0.48928500
C -3.13488400 -0.95448400 -0.66746900
C -1.89631100 -0.53256200 -1.12640000
H -1.17242400 1.73501600 1.29517000
H -3.38978700 0.99570200 2.08861900
H -4.65224000 -0.73470400 0.84134800
H -3.68109900 -1.70829500 -1.22295800
H -1.46678000 -0.94228400 -2.03306000
N 0.09591900 0.75091100 -0.90962000
N 0.74995700 1.69170600 -0.36501100
N 1.86334700 1.91549300 -0.12266100

CA-30
E= -591.155288 a.u.

C 2.58303900 -0.95956900 1.20628000
C 1.53190000 -1.60578200 0.29856300
C 1.20288400 -0.50903000 -0.73202900
C 2.43198200 0.43134900 -0.75967100
C 3.44772300 -0.15907600 0.22825600
H 3.15384600 -1.69011200 1.78174600
H 0.64480200 -1.94800100 0.83414600
H 1.96177100 -2.46727700 -0.22346500
H 0.92510000 -0.90803900 -1.71032100
H 2.85678400 0.59880300 -1.75025300
H 4.03762100 0.62723100 0.70095400
H 4.13302300 -0.82624700 -0.30417700
H 2.09772800 -0.28241900 1.91639200
C -1.17556600 0.18892200 -0.11898800
C -2.02266700 1.16754500 0.41363800
C -3.37572300 0.90630800 0.54867500
C -3.91258000 -0.31935200 0.16616300
C -3.07035000 -1.28666400 -0.36110900
C -1.71026400 -1.04227400 -0.50656700
H -1.60775900 2.12109800 0.70937300
H -4.02001400 1.67457300 0.96140200
H -4.97220400 -0.51452100 0.27839200
H -3.46871400 -2.24743800 -0.66735800
H -1.07207900 -1.81163100 -0.92285000
N 0.19094100 0.43208600 -0.26664000
N 0.70962000 1.66315200 -0.02062500
N 1.92055600 1.73329200 -0.27034300

31
E = -234.632667028 a.u.

C -0.37568600 -0.66566700 -1.18626500
C 0.37568600 0.66566700 -1.18626500
C 0.00571200 1.49568800 0.04500600
C -0.00571200 0.66496300 1.30072300
C 0.00571200 -0.66496300 1.30072300

C -0.00571200 -1.49568800 0.04500600
H 0.70560500 2.32958000 0.16376900
H 1.45394800 0.46644800 -1.17535900
H 0.16497700 1.22894000 -2.09953200
H -1.45394800 -0.46644800 -1.17535900
H -0.16497700 -1.22894000 -2.09953200
H 0.98300200 -1.95360100 -0.09346500
H -0.70560500 -2.32958000 0.16376900
H -0.98300200 1.95360100 -0.09346500
H 0.02051400 -1.19781400 2.24780400
H -0.02051400 1.19781400 2.24780400

TS-31
E = -630.381209794 a.u.
Freq = -479.58i cm^{-1}

N -1.51952600 2.13600800 0.29398900
N 0.21263300 1.06693500 -0.65853000
N -0.39943600 1.89177100 0.08919300
C -1.52374400 -0.13190900 -1.26350000
C -2.53322100 0.59832100 -0.65028500
C 1.45359700 0.55549800 -0.24961100
C 1.95959600 0.68571100 1.04662200
C 2.17209200 -0.17313100 -1.19898900
C 3.17094900 0.09671800 1.37660400
C 3.37331600 -0.77406000 -0.85197200
C 3.88054200 -0.64087600 0.43514800
H 1.40571300 1.25631800 1.78325800
H 3.56070700 0.21105500 2.38183300
H 4.82336900 -1.10328700 0.70185100
H 3.92143000 -1.34027400 -1.59638400
H 1.77698300 -0.25436400 -2.20499200
C -1.46919800 -1.66868000 0.71569800
C -2.95890200 -1.38528600 0.90142400
C -3.30159900 0.06722500 0.55014700
C -1.09338700 -1.48095200 -0.75057300
H -4.37336200 0.15373600 0.34801700
H -3.52222600 -2.06523300 0.25098900
H -3.27252900 -1.59918700 1.92664000
H -0.87511000 -0.98594600 1.33582300
H -1.22526800 -2.68435900 1.03779700
H -1.59670300 -2.24767100 -1.35576300
H -0.02157300 -1.63069100 -0.90304600
H -3.10630800 0.70877300 1.41566100
H -1.28282400 0.09698100 -2.29459800
H -3.04823600 1.32967000 -1.26395000

CA-31
E = -630.467314050 a.u.

N -1.51952600 2.13600800 0.29398900
N 0.21263300 1.06693500 -0.65853000
N -0.39943600 1.89177100 0.08919300

C -1.52374400 -0.13190900 -1.26350000
C -2.53322100 0.59832100 -0.65028500
C 1.45359700 0.55549800 -0.24961100
C 1.95959600 0.68571100 1.04662200
C 2.17209200 -0.17313100 -1.19898900
C 3.17094900 0.09671800 1.37660400
C 3.37331600 -0.77406000 -0.85197200
C 3.88054200 -0.64087600 0.43514800
H 1.40571300 1.25631800 1.78325800
H 3.56070700 0.21105500 2.38183300
H 4.82336900 -1.10328700 0.70185100
H 3.92143000 -1.34027400 -1.59638400
H 1.77698300 -0.25436400 -2.20499200
C -1.46919800 -1.66868000 0.71569800
C -2.95890200 -1.38528600 0.90142400
C -3.30159900 0.06722500 0.55014700
C -1.09338700 -1.48095200 -0.75057300
H -4.37336200 0.15373600 0.34801700
H -3.52222600 -2.06523300 0.25098900
H -3.27252900 -1.59918700 1.92664000
H -0.87511000 -0.98594600 1.33582300
H -1.22526800 -2.68435900 1.03779700
H -1.59670300 -2.24767100 -1.35576300
H -0.02157300 -1.63069100 -0.90304600
H -3.10630800 0.70877300 1.41566100
H -1.28282400 0.09698100 -2.29459800
H -3.04823600 1.32967000 -1.26395000

34
E = -345.764878 a.u.

C 1.18641200 0.03355200 0.00010300
C 2.10696400 -0.92678200 -0.00033900
H 3.16563300 -0.69209700 -0.00079400
H 1.81024600 -1.96887900 -0.00023700
C 1.49882600 1.50271200 -0.00000800
H 1.06939000 1.99323200 -0.87697900
H 1.07024200 1.99317300 0.87741100
H 2.57787100 1.66485600 -0.00052600
C -0.24735600 -0.40037600 0.00078100
O -0.63262300 -1.54055400 0.00004400
O -1.07868000 0.65343800 0.00020000
C -2.46997100 0.33911100 -0.00040400
H -2.98791300 1.29556400 -0.00204100
H -2.73151000 -0.24032600 -0.88755800
H -2.73277800 -0.23789400 0.88797400

TS-34-o
E= -741.524004 a.u.
Freq = 487.30i cm^{-1}

C -0.80165900 -1.06575600 -1.05627300
H -0.55922900 -2.05104400 -1.43570400
H -0.32860600 -0.22700600 -1.55048500

C -1.99917800 -0.88364300 -0.38245000
C 1.85710200 -0.49475700 0.23633300
C 2.66079400 -1.00234000 -0.78255500
C 2.27775100 0.61346300 0.97151800
N 0.60917200 -1.12587200 0.42881000
C 3.87664200 -0.39868900 -1.06754300
C 3.50459700 1.19658000 0.68996500
N -0.09895700 -0.81231600 1.43224400
C 4.30623000 0.69905300 -0.33095400
N -1.21923400 -0.68113800 1.68054500
H 2.32462100 -1.86951200 -1.33852300
H 1.64719800 1.00894900 1.75924800
H 4.49626000 -0.79590500 -1.86314400
H 3.83197100 2.05177000 1.26998600
H 5.26079500 1.16270300 -0.54917800
C -2.95797700 -2.02224100 -0.14489700
H -3.54860500 -1.85487400 0.75588000
H -3.65719800 -2.11820900 -0.98062900
H -2.41345000 -2.96304200 -0.03905200
C -2.58362500 0.47774500 -0.29878700
O -3.74790500 0.70996700 -0.09733600
O -1.65893800 1.44526100 -0.46111400
C -2.14978100 2.78025400 -0.37944400
H -1.28409000 3.42194600 -0.53002900
H -2.90021300 2.96457400 -1.15042400
H -2.59695500 2.96508700 0.59898700

TS-34-m
E = -741.527565 a.u.
Freq =484.90i cm^{-1}

C 2.95115400 -0.34206600 -0.42880900
H 2.98763700 -0.27718000 -1.50821300
H 3.86791100 -0.62247900 0.07728000
C 2.02063200 0.43087800 0.25022900
C -0.84511900 -0.95083100 0.41390200
C -1.56668200 -0.28807800 1.40500100
C -1.45320800 -1.26811000 -0.80142400
N 0.52597100 -1.16474100 0.66482400
C -2.89196600 0.05416700 1.18205200
C -2.78436900 -0.93828000 -1.00777500
N 1.14255400 -2.06697300 0.02268000
C -3.50615500 -0.27303000 -0.02209000
N 2.19177300 -2.18925600 -0.46804500
H -1.07347500 -0.04814700 2.33891400
H -0.87811500 -1.75754900 -1.57851000
H -3.44972400 0.57058800 1.95468700
H -3.25649500 -1.19089000 -1.95006600
H -4.54441400 -0.01280200 -0.19167600
C 1.02482200 1.14444400 -0.59915100
C 2.23379300 0.86133700 1.67615100
H 2.80986600 1.79177600 1.70646800
H 1.28966400 1.03912700 2.18835800
H 2.79015500 0.09574000 2.21969900
O 0.84667000 0.93142300 -1.77339100

O 0.30504600 2.02740700 0.10474000
C -0.78425700 2.62773400 -0.59685600
H -1.24176700 3.31790800 0.10844800
H -0.42734500 3.15909100 -1.48018500
H -1.50156700 1.86197400 -0.89958900

CA-34-o
E= -741.596121 a.u.

C -0.43212100 -0.29679900 -0.92961600
H -0.18679600 -0.89276700 -1.81223800
H -0.51853900 0.75576500 -1.21179100
C -1.67815000 -0.83415800 -0.20209800
C 1.91733500 -0.11738900 0.02577000
C 2.42340200 0.37855900 -1.17661300
C 2.76843100 -0.26663800 1.12569700
N 0.56811500 -0.46796500 0.11217300
C 3.76678300 0.72087800 -1.27416400
C 4.10339500 0.08169200 1.00965900
N 0.01157300 -0.83486900 1.28559400
C 4.61485100 0.57637700 -0.18668300
N -1.20791700 -1.03439900 1.20672700
H 1.77640000 0.49987500 -2.03666200
H 2.37090600 -0.65031900 2.05516400
H 4.14663500 1.10485200 -2.21412900
H 4.75391500 -0.03673000 1.86886200
H 5.66127600 0.84470900 -0.26681800
C -2.16909700 -2.17181700 -0.73506300
H -2.96715800 -2.55840100 -0.10214700
H -2.55648900 -2.06006800 -1.74985700
H -1.34265600 -2.88603400 -0.74215800
C -2.81845900 0.18011000 -0.14238000
O -3.96146800 -0.05253600 -0.42132400
O -2.37542500 1.36723200 0.27838200
C -3.36847600 2.38307400 0.43420600
H -2.83458100 3.26359600 0.78289200
H -3.86278500 2.58329700 -0.51777400
H -4.11474900 2.07195000 1.16646100

CA-34-m
E = -741.594016 a.u.

C 1.98503900 -1.88616900 0.01651300
H 2.55981500 -1.74445800 -0.90180200
H 2.64655100 -2.24406000 0.80573600
C 1.20647600 -0.61376500 0.41760100
C -1.30956200 -0.27913600 -0.03534800
C -1.29977300 1.08199400 0.27622100
C -2.52754700 -0.90411700 -0.32447000
N -0.11393100 -1.01299500 -0.08497600
C -2.48947200 1.79925600 0.30185800
C -3.70314300 -0.17252300 -0.29604000
N -0.15843800 -2.35139400 -0.33770900
C -3.69805100 1.18241400 0.01762600
N 0.94967500 -2.89249800 -0.26651600

H -0.37532400 1.59604300 0.50316900
H -2.53666500 -1.95620300 -0.57114100
H -2.46074200 2.85492000 0.54724600
H -4.63750700 -0.67321500 -0.52351900
H -4.62256100 1.74662400 0.03764300
C 1.73209400 0.57052500 -0.40257900
C 1.19956500 -0.40522100 1.93212400
H 2.20845000 -0.18743200 2.28693200
H 0.54662200 0.41219400 2.23483400
H 0.84936100 -1.32366000 2.40909900
O 1.85056800 0.55080600 -1.59514100
O 2.05791600 1.61691300 0.36252200
C 2.54250000 2.76423900 -0.34170800
H 2.76723700 3.50375500 0.42287500
H 3.43847300 2.51136600 -0.90995700
H 1.77851100 3.13560300 -1.02655400

37
E =-306.446664 a.u.

C 2.15775100 -0.76554000 -0.00011600
C 1.48840300 0.38042800 0.00002300
H 3.24171000 -0.77943100 -0.00017700
H 1.63968400 -1.71730900 -0.00016800
H 1.99050000 1.34100100 0.00007900
C 0.00817800 0.48478900 0.00012900
O -0.58333000 1.53328900 0.00019900
O -0.60205900 -0.70940400 -0.00006900
C -2.02794400 -0.66958200 -0.00010800
H -2.35133500 -1.70813000 -0.00062100
H -2.39792100 -0.15432800 0.88813500
H -2.39785900 -0.15344800 -0.88786100

TS-37-o
E=-702.207597 a. u.
Freq = 491.70i cm^{-1}

C -0.89215300 -1.30858400 -1.15982900
H -0.59527900 -2.26724300 -1.56523900
H -0.46790100 -0.43149000 -1.63335700
C -2.09834100 -1.20484200 -0.49075000
C 1.65407400 -0.51743600 0.20122000
C 2.53358100 -0.85789100 -0.82387400
C 1.91404700 0.58965300 1.00816700
N 0.49082600 -1.31046100 0.32614400
C 3.66693500 -0.08854300 -1.04310700
C 3.06082100 1.33957000 0.79201800
N -0.24898600 -1.16896400 1.34530800
C 3.93814700 1.00890300 -0.23445600
N -1.37462400 -1.18657200 1.60198800
H 2.32148300 -1.72646600 -1.43603800
H 1.22208200 0.85576900 1.79866900
H 4.34691400 -0.35563200 -1.84367700
H 3.26497300 2.19389500 1.42706800
H 4.82905800 1.60230800 -0.40162000

C -2.78672300 0.08915500 -0.31921900
O -3.96112500 0.22226500 -0.09513200
O -1.93257100 1.12891500 -0.42696600
C -2.51652100 2.41905900 -0.26963900
H -1.69937900 3.12834900 -0.38408600
H -3.28138300 2.59245400 -1.02889500
H -2.97193100 2.51629200 0.71761300
H -2.73278700 -2.06995700 -0.35091100

TS-37-m
E = -702.211094 a.u.
Freq =485.22i cm^{-1}

C -3.15029700 -0.01914400 -0.06276300
H -3.35303100 0.19824400 0.97860800
H -3.99572900 -0.30418400 -0.67668000
C -2.05378100 0.58180600 -0.65480800
C 0.64608400 -0.99388100 -0.36141300
C 1.51995500 -0.50834600 -1.33147300
C 1.09177700 -1.20341800 0.94369400
N -0.70495200 -1.14799200 -0.74539000
C 2.83853500 -0.23880900 -0.99769300
C 2.41690100 -0.94689700 1.26347900
N -1.45937900 -1.90558500 -0.06561300
C 3.29233000 -0.46097100 0.29817800
N -2.55803100 -1.88548600 0.32031900
H 1.14738400 -0.34056400 -2.33427300
H 0.39938300 -1.55512400 1.69943800
H 3.51619700 0.14004700 -1.75395500
H 2.76351600 -1.11638300 2.27621000
H 4.32519300 -0.25719200 0.55527800
C -1.11636300 1.35494900 0.19014900
O -1.09595600 1.33434500 1.39583800
O -0.24741200 2.04838900 -0.55693500
C 0.80884300 2.68352100 0.16469800
H 1.40029600 3.20787900 -0.58244700
H 0.40793700 3.38332300 0.89929300
H 1.41832300 1.93319500 0.67328500
H -1.98989200 0.72947200 -1.72347900

CA-37-o
E = -702.276824 a.u.

C 0.54656500 -0.07497500 -1.17502700
H 0.22232800 0.03205400 -2.21326600
H 0.68097200 -1.13394500 -0.94279600
C 1.78785400 0.76749200 -0.85378200
C -1.74603300 0.15228900 -0.09178100
C -2.26512300 -0.89596200 -0.85299200
C -2.56526300 0.80884100 0.83237600
N -0.41359500 0.53307500 -0.26423400
C -3.59059000 -1.28040800 -0.68948600
C -3.88316300 0.41136800 0.98087600
N 0.13378200 1.53342300 0.45218300
C -4.40767100 -0.63294700 0.22468800

N 1.32756600 1.73403500 0.18755100
H -1.64288700 -1.41436900 -1.57210300
H -2.15746200 1.61963300 1.42011500
H -3.98103400 -2.09608000 -1.28733900
H -4.50949200 0.92700600 1.70004100
H -5.44027500 -0.93569800 0.34903300
C 2.96174500 -0.01153900 -0.28410500
O 4.09529400 0.09018800 -0.66005600
O 2.56055200 -0.81561900 0.70383600
C 3.59098100 -1.55993800 1.35802500
H 3.08867300 -2.14274000 2.12605900
H 4.09875500 -2.21412500 0.64750300
H 4.31962800 -0.88243000 1.80508200
H 2.16394900 1.33508200 -1.70382800

CA-37-m
E = -702.278612 a.u.

C -2.04060500 -1.89056600 -0.51616300
H -2.80920000 -1.83110400 0.25732400
H -2.50034500 -2.20383900 -1.45293700
C -1.23827400 -0.58133100 -0.63123400
C 1.23041700 -0.30889500 -0.06423900
C 1.26737000 0.99585600 -0.55803100
C 2.39130400 -0.88085600 0.46604300
N 0.03355700 -1.03567000 -0.09000700
C 2.45631000 1.71560200 -0.52118000
C 3.56633900 -0.14933600 0.48994700
N 0.03542500 -2.38047000 0.13111400
C 3.61088900 1.15254700 -0.00034700
N -1.05778300 -2.90664500 -0.09325500
H 0.37953700 1.45852500 -0.97054600
H 2.35698100 -1.89158100 0.84816900
H 2.47057200 2.72812600 -0.90846600
H 4.45997000 -0.60407400 0.90227000
H 4.53454500 1.71793800 0.02632600
C -1.84069600 0.52268100 0.23062400
O -2.09462300 0.40411700 1.39535400
O -2.06580200 1.62830500 -0.48569700
C -2.61921300 2.73046300 0.24101200
H -2.75450900 3.52468700 -0.48887200
H -3.57396200 2.44997900 0.68771200
H -1.93292600 3.04335100 1.02917500
H -1.12870300 -0.22888000 -1.66095800

39
E = -305.177897808 a.u.

C -2.62232400 -0.40694200 -0.00015300
C -1.45992100 -0.11813400 0.00015000
C -0.07073500 0.30625500 -0.00000900
O 0.27986000 1.45362800 -0.00002700
O 0.74924600 -0.74567600 -0.00010200
C 2.14495200 -0.43072400 0.00006000
H 2.40576500 0.14526600 0.88929400

H 2.65750900 -1.38932600 -0.00037300
H 2.40590100 0.14605600 -0.88864200
H -3.65384900 -0.66833600 0.00045400

TS-39-o
E= -700.936317571 a.u.
Freq = 480.83i cm^{-1}

N 1.04324500 -1.24535800 -0.91254200
N -0.04109800 -0.87163000 -0.99618100
N -0.72598100 0.15446700 -0.74705100
C 0.67689200 1.18275500 0.34996000
C 1.71038400 0.51883900 0.28047300
C 3.07442500 0.10844000 0.55856700
O 3.41831800 -0.47500300 1.55012800
O 3.89060300 0.45477900 -0.44256100
C 5.25603800 0.06982800 -0.27219600
H 5.33894500 -1.01460400 -0.18300800
H 5.76932400 0.42036700 -1.16442400
H 5.67844900 0.53411300 0.62055100
C -2.07524300 0.03860300 -0.34328400
C -2.83474400 1.20563100 -0.37495000
C -2.63573500 -1.15158900 0.11912700
C -4.14999800 1.18314700 0.06634500
C -3.95775800 -1.16594500 0.53829300
C -4.71731200 -0.00142400 0.52028800
H -2.38865600 2.11633500 -0.75722100
H -2.03977100 -2.05664000 0.14502800
H -4.73726500 2.09366100 0.04260400
H -4.39410100 -2.09385300 0.88932200
H -5.74751500 -0.01894000 0.85511700
H 0.03436500 1.98927600 0.62616900

TS-39-m
E = -700.938337452 a.u.
Freq = -511.73i cm^{-1}

N -1.90449300 -2.72528100 -0.11572000
N -0.90303200 -2.27983200 0.26103200
N -0.44643500 -1.16786000 0.61380400
C -2.18179900 -0.06624300 -0.11207900
C -2.95423200 -0.97442700 -0.41369200
C -1.62368800 1.25825400 0.11691600
O -1.68840500 1.86333700 1.15238200
O -1.00022400 1.69232000 -0.98140800
C -0.34481600 2.95674500 -0.85593000
H 0.06303800 3.16922700 -1.84097700
H -1.05352500 3.72960600 -0.55534800
H 0.45725000 2.89231500 -0.11859800
C 0.88865600 -0.79733100 0.35395300
C 1.37478700 0.29400500 1.07141900
C 1.68626700 -1.42386000 -0.60311100
C 2.65434100 0.76646400 0.81670500
C 2.97066300 -0.95449600 -0.83336600
C 3.45698400 0.14380800 -0.13209500

H 0.73865700 0.75919700 1.81503400
H 1.30048000 -2.27159400 -1.15764500
H 3.03027700 1.61644600 1.37457500
H 3.59337500 -1.44671900 -1.57141900
H 4.45990600 0.50790100 -0.32092100
H -3.86568800 -1.40834400 -0.75862100

CA-39-o
E = -701.087488191 a.u.

N 1.23549400 -1.37564700 -0.34363300
N -0.04524000 -1.46885500 -0.37353200
N -0.55880700 -0.25110900 -0.07595100
C 0.43094000 0.63350800 0.14819400
C 1.57825800 -0.09714500 -0.02846300
C 2.94969800 0.42397400 0.11235000
O 3.18435900 1.57309100 0.39245800
O 3.87517000 -0.50597500 -0.10176900
C 5.22777500 -0.06482000 0.01864700
H 5.42005800 0.31054100 1.02519300
H 5.83795800 -0.94090400 -0.18643300
H 5.43794800 0.72716500 -0.70219500
C -1.96585300 -0.05134600 -0.02805500
C -2.49822000 1.18941700 -0.35604300
C -2.78690100 -1.10750100 0.34838200
C -3.87197700 1.37777700 -0.28732500
C -4.15904800 -0.90969000 0.39729100
C -4.70449300 0.33094300 0.08753100
H -1.85077900 1.99525200 -0.68067200
H -2.34394300 -2.06474500 0.58859000
H -4.29096200 2.34412500 -0.54128600
H -4.80431600 -1.73032300 0.68738400
H -5.77664400 0.48011800 0.13373800
H 0.27324400 1.66041500 0.42692400

CA-39-m
E = -701.082750888 a.u.

N -1.65106800 -2.74515700 0.10511700
N -0.39226100 -2.44036400 0.07960100
N -0.28111900 -1.10539200 0.05294600
C -1.51893700 -0.53322100 0.07027200
C -2.37578200 -1.60626800 0.10744000
C -1.89679000 0.88834900 -0.03395600
O -3.02427500 1.27052000 0.13087200
O -0.87062700 1.67650900 -0.35563800
C -1.17111300 3.06803400 -0.48487000
H -0.22319000 3.54762200 -0.71555900
H -1.88993300 3.22809400 -1.28969600
H -1.58478600 3.45695100 0.44667400
C 1.02388900 -0.52470600 0.06671500
C 1.38249200 0.35004200 1.08245500
C 1.92413200 -0.88788500 -0.92318300
C 2.66176000 0.88536900 1.09227000
C 3.20587800 -0.35426200 -0.89931800

C 3.57360700 0.53543200 0.10220500
H 0.66764500 0.60069000 1.85632700
H 1.61742800 -1.58557800 -1.69189500
H 2.95059700 1.56907300 1.88170700
H 3.91660100 -0.63412700 -1.66769500
H 4.57401000 0.95187900 0.11643100
H -3.45285100 -1.59975100 0.11801300

40
E = -170.808643 a.u.

C 1.59576400 -0.36036000 0.00003200
H 2.62134800 -0.01227200 -0.00024600
H 1.42483500 -1.43032500 0.00027900
C 0.58813300 0.50681600 -0.00006200
H 0.75924700 1.57749200 0.00053600
C -0.78181200 0.09343000 -0.00014700
N -1.88827700 -0.22488800 0.00007100

TS-40-o
E = -566.567301 a.u.
Freq = 502.65i cm^{-1}

C 1.54337400 1.39372200 -0.35034700
H 1.39112300 2.38043000 0.06609600
H 0.99816800 1.17044900 -1.26022300
C 2.73828800 0.73804100 -0.08789900
H 3.48137100 1.18671200 0.55832000
C 3.19955900 -0.29462800 -0.95974900
N 3.55991900 -1.12954500 -1.66798500
C -1.07469300 0.16545400 0.38972200
C -1.88206500 1.21736800 -0.03596000
C -1.52774700 -1.14983700 0.29967600
N 0.21566700 0.50851500 0.85862700
C -3.13891700 0.95090900 -0.55919000
C -2.79449200 -1.40146500 -0.20673700
N 0.93060400 -0.36262500 1.43746200
C -3.60156200 -0.35694500 -0.64248100
N 2.04683700 -0.64036400 1.52589600
H -1.52006400 2.23484500 0.05293500
H -0.89405700 -1.96570600 0.62755100
H -3.76327400 1.77138700 -0.89285100
H -3.14796100 -2.42401500 -0.26877300
H -4.58696200 -0.56169900 -1.04326600

TS-40-m
E = -566.565754 a.u.
Freq = 489.62i cm^{-1}

C 3.16520300 0.16046300 -0.06790900
H 3.42734200 0.24997800 -1.11388300
H 3.96413200 -0.13243400 0.60169900
C 2.11673500 0.91456400 0.44262000
C -0.69495200 -0.48510400 0.38723400
C -1.44762300 0.32401500 1.23394200

C -1.25898800 -1.00083400 -0.77889200
N 0.65855100 -0.67933000 0.74248600
C -2.76331500 0.61952400 0.91171700
C -2.58150400 -0.71495700 -1.08091400
N 1.33926500 -1.57113000 0.16365300
C -3.33562500 0.09772200 -0.24215600
N 2.42573200 -1.68824300 -0.24045000
H -0.98989700 0.71625200 2.13419300
H -0.66577400 -1.62440200 -1.43781100
H -3.34506400 1.25602500 1.56783300
H -3.02186900 -1.12158800 -1.98373100
H -4.36569500 0.32528800 -0.48908600
C 1.32891800 1.74173500 -0.41749300
N 0.68308000 2.39936200 -1.10885800
H 2.07733300 1.16351000 1.49407100

CA-40-o
E = -566.634637 a.u.

C 1.25684100 -0.81082400 -0.45546200
H 1.08844600 -1.40358400 -1.35428600
H 1.24637800 -1.46572200 0.42231700
C 2.53050000 0.04315500 -0.54214200
H 2.89099600 0.13478900 -1.57104500
C 3.62710800 -0.43896800 0.28951700
N 4.47768000 -0.84926000 0.94362100
C -1.10293900 0.06621800 -0.11390800
C -1.63757900 -1.21981800 -0.17530300
C -1.93900200 1.15694700 0.13774400
N 0.27162600 0.25457600 -0.32779200
C -3.00081100 -1.41085200 0.01759100
C -3.29412900 0.94684800 0.33025000
N 0.85779400 1.43576900 -0.04178000
C -3.83594200 -0.33371900 0.27131600
N 2.09393500 1.41142500 -0.11501700
H -1.00184200 -2.07449100 -0.37170400
H -1.51716700 2.15148000 0.18502800
H -3.40539800 -2.41517100 -0.03130800
H -3.93535700 1.79805100 0.52820700
H -4.89759500 -0.48683900 0.42193800

CA-40-m
E = -566.634397 a.u.

C 2.90676400 -0.44981700 0.50287800
H 3.73429800 -0.02319800 -0.06090200
H 3.26156700 -0.72728200 1.49769000
C 1.66851300 0.46791700 0.57192200
C -0.73931700 -0.25757700 0.11938800
C -1.26104400 0.96784300 0.53155300
C -1.59526100 -1.25212400 -0.36006800
N 0.64184300 -0.49659100 0.20798100
C -2.63033100 1.19351500 0.46169600
C -2.95722700 -1.00839700 -0.42256200
N 1.19411700 -1.64343100 -0.27918700

C -3.48601400 0.21146000 -0.01321600
N 2.42325400 -1.67405800 -0.16486900
H -0.61377300 1.75645500 0.89516800
H -1.18450000 -2.19999300 -0.67876000
H -3.02270900 2.15212900 0.78043700
H -3.61314400 -1.78546600 -0.79794000
H -4.55252500 0.39275400 -0.06731000
C 1.74286200 1.60059900 -0.36750300
N 1.82617700 2.48975000 -1.09079000
H 1.49937300 0.86440200 1.57514100

41
E = -533.037151 a.u.

C 0.59681100 -0.19548200 0.06196700
C -0.59678800 -0.19546100 -0.06199800
C -2.03213700 -0.24863200 -0.28072200
O -2.55285200 -0.96654900 -1.08756700
O -2.66639500 0.59742200 0.52747400
C -4.09226900 0.61948800 0.39182900
H -4.50954400 -0.36433100 0.61095000
H -4.43863000 1.35383200 1.11422100
H -4.37287400 0.91163200 -0.62107300
C 2.03214700 -0.24870500 0.28064600
O 2.55282000 -0.96685300 1.08731600
O 2.66639200 0.59754600 -0.52731100
C 4.09228000 0.61960300 -0.39168000
H 4.43860000 1.35426900 -1.11376200
H 4.37289100 0.91130900 0.62134400
H 4.50957200 -0.36410900 -0.61123700

TS-41
E = -928.798610 a.u.
Freq = 461.72i cm^{-1}

N 1.44441100 -2.01728700 -0.28457600
N 0.33143200 -1.85714200 -0.54248600
N -0.46320300 -0.91753400 -0.78918200
C 0.82426500 0.62216500 -0.18320600
C 1.89760000 0.05707000 0.03420700
C 3.28545400 -0.03787400 0.47037700
O 3.63549000 0.01915500 1.61652400
O 4.09941000 -0.20906900 -0.57190600
C 5.48658600 -0.33276000 -0.24773200
H 5.65022500 -1.19417600 0.40165900
H 5.99477300 -0.46781800 -1.19921900
H 5.84430200 0.56742900 0.25461200
C -0.12319300 1.72943000 -0.29615500
O -0.31501200 2.36713000 -1.29453700
O -0.76522900 1.90222300 0.85874900
C -1.78117900 2.90902200 0.85379200
H -2.16672400 2.93407500 1.86970100
H -1.36138300 3.87617900 0.57447600
H -2.57223100 2.63856900 0.15216200
C -1.81749600 -0.96813100 -0.38615700

C -2.69291100 -0.12006200 -1.05924700
C -2.26706600 -1.75848800 0.66995600
C -4.02148300 -0.05512700 -0.66289500
C -3.60130200 -1.70013200 1.04254000
C -4.47985900 -0.84557500 0.38427700
H -2.31775700 0.48097600 -1.87898000
H -1.57547900 -2.40951000 1.19236600
H -4.70323200 0.60585900 -1.18545900
H -3.95479500 -2.31966200 1.85842100
H -5.51994500 -0.80091700 0.68478500

CA-41
E = -928.942747 a.u.

N 0.76831700 -2.42191100 -0.00636300
N -0.50445800 -2.26640600 -0.03406600
N -0.76644000 -0.93957500 -0.09516200
C 0.38807100 -0.23793100 -0.09385500
C 1.36737400 -1.20433700 -0.04124100
C 2.83579800 -1.04928600 -0.03959700
O 3.62720400 -1.92432900 0.16172700
O 3.16719400 0.22629800 -0.30517500
C 4.56648400 0.50850800 -0.31043300
H 5.07539400 -0.09845700 -1.06060700
H 4.65208800 1.56512200 -0.55348100
H 5.00123600 0.30313800 0.66922600
C 0.48942000 1.24989600 -0.13701400
O 0.20900500 1.91936600 -1.09293900
O 0.93087900 1.71863200 1.02220200
C 1.15880300 3.13095900 1.06785100
H 1.52292100 3.33308300 2.07161500
H 1.90325000 3.41332200 0.32207000
H 0.23166800 3.67255500 0.87614300
C -2.12129400 -0.48817000 -0.07961300
C -2.99040100 -1.04722700 0.84946400
C -2.55164600 0.46505300 -0.99321800
C -4.31465400 -0.63558900 0.86529600
C -3.87723700 0.87809600 -0.95511200
C -4.75796700 0.33058800 -0.03107100
H -2.62448200 -1.79955800 1.53609700
H -1.85998400 0.87518500 -1.71718200
H -5.00033200 -1.06839100 1.58384400
H -4.22195000 1.62343300 -1.66180300
H -5.79251000 0.65271500 -0.01203500

15
E = -283.068767 a.u.

C 1.86158100 0.05385900 -0.00001000
H 1.83436500 1.13636400 0.00000600
H 2.81795800 -0.45284900 -0.00003200
C 0.74269000 -0.64382700 0.00000700
H 0.63972300 -1.71884300 -0.00000700
N -0.56134600 0.03167600 0.00005400
O -1.53138900 -0.70014900 -0.00002500

O -0.59214200 1.24432500 -0.00001600

TS-15-o
E = -678.831833 a.u.
Freq = 509.75i cm^{-1}

C -1.15594500 -0.89031100 -1.24226800
H -1.01623400 -1.84083200 -1.73906400
H -0.60702800 -0.04183300 -1.63220300
C -2.35733400 -0.66260800 -0.60725500
H -3.18966600 -1.34753800 -0.57650500
C 1.36736600 -0.47441900 0.15713200
C 2.47151600 -1.10325500 -0.40366500
C 1.42735800 0.85932000 0.55456300
N 0.14702100 -1.21408900 0.21920800
C 3.65694200 -0.39500200 -0.55276300
C 2.61998300 1.55300800 0.41460500
N -0.59094000 -1.06934500 1.24023700
C 3.73394500 0.92903700 -0.13849900
N -1.70422500 -0.97642600 1.51407900
H 2.39224400 -2.14008900 -0.70754800
H 0.54013300 1.34634100 0.94353900
H 4.52275300 -0.88116200 -0.98655100
H 2.67538200 2.58923400 0.72631800
H 4.66126200 1.47843200 -0.25075800
N -2.74445800 0.70691300 -0.32924000
O -3.92259900 0.91844700 -0.12560800
O -1.86660200 1.55823500 -0.29668100

TS-15-m
E = -678.830312 a.u
Freq = 491.44i cm^{-1}

C -3.02787800 -0.09740600 -0.00905300
H -3.22109700 -0.05222300 1.05409000
H -3.85425900 -0.35862400 -0.65697900
C -2.01196500 0.67208100 -0.52961100
C 0.81984900 -0.60515000 -0.44239400
C 1.59332400 0.20662100 -1.26722800
C 1.32674300 -1.07105200 0.77062800
N -0.50776600 -0.84968800 -0.86418900
C 2.88104900 0.54579500 -0.88042500
C 2.62129700 -0.74051700 1.13768900
N -1.17367400 -1.77720400 -0.32508300
C 3.39971600 0.06880100 0.31700600
N -2.25700300 -1.94499700 0.06343700
H 1.17326600 0.56667800 -2.19805500
H 0.70939300 -1.68522200 1.41562900
H 3.48119300 1.18303500 -1.51870100
H 3.01999800 -1.10739500 2.07601900
H 4.40830100 0.33052600 0.61413300
H -1.96975600 1.04585600 -1.53969800
N -1.17979700 1.45524800 0.37650200
O -0.56075200 2.37707300 -0.11957000

O -1.13077100 1.12527900 1.54697100

CA-15-o
E = -678.901201 a.u.

C 0.90163900 -0.75073000 -0.73982000
H 0.65851100 -1.12414200 -1.73696500
H 0.93782800 -1.57328500 -0.02358200
C 2.18102300 0.06835500 -0.72735200
H 2.76484100 0.07184700 -1.64350800
C -1.42538500 0.08888500 -0.11597500
C -1.98557500 -1.17190500 -0.31324500
C -2.23195000 1.15919700 0.27679600
N -0.04875100 0.26839400 -0.31796300
C -3.34911500 -1.35761400 -0.11967200
C -3.58863800 0.95474500 0.46490000
N 0.54071200 1.45166800 -0.14462200
C -4.15748100 -0.30003100 0.26866400
N 1.76734300 1.44162600 -0.36952800
H -1.36864100 -2.01046400 -0.61217500
H -1.78771200 2.13297800 0.43067300
H -3.77549200 -2.34193200 -0.27428300
H -4.20888600 1.78939000 0.77057800
H -5.21965000 -0.44924600 0.41950700
N 3.15293000 -0.37278500 0.35748100
O 4.32384000 -0.18371500 0.13068400
O 2.68196600 -0.83664500 1.37261600

CA-15-m
E = -678.905548 a.u.

C -2.62616100 -0.85922500 -0.62148000
H -3.48536000 -0.50921300 -0.05020700
H -2.95885000 -1.13506400 -1.62376600
C -1.47010800 0.14132100 -0.66190500
C 0.95639200 -0.32477600 -0.15217500
C 1.34966800 0.96874800 -0.49119700
C 1.90465900 -1.25473100 0.27541800
N -0.39684000 -0.69324600 -0.26010900
C 2.68989000 1.32469400 -0.40333600
C 3.23564100 -0.87995300 0.36065800
N -0.84386100 -1.91339300 0.18855600
C 3.63896400 0.40719000 0.02120800
N -2.05646900 -2.05591000 0.02232900
H 0.62695100 1.70950700 -0.81270900
H 1.58929200 -2.25452300 0.53962600
H 2.98485000 2.33378000 -0.66619800
H 3.96617600 -1.60670400 0.69672200
H 4.68197600 0.69088800 0.09118700
H -1.31719700 0.65719400 -1.60762800
N -1.71386100 1.27150400 0.35594800
O -1.97336600 2.36010400 -0.10992800
O -1.66217200 0.97887700 1.52527300

5
E = -78.5795263528 a.u.

C -0.66214800 0.00000000 0.00000400
C 0.66214800 0.00000000 -0.00000300
H -1.23144700 -0.92379300 -0.00001100
H -1.23144700 0.92379300 0.00002200
H 1.23144700 0.92379300 0.00001000
H 1.23144700 -0.92379300 -0.00002400

TS-5
E = -474.33716014 a.u.
Freq = -475.71i cm^{-1}

N 2.64135900 -1.32951600 -0.16442000
N 1.54571000 -1.05640200 -0.43434800
N 0.85172700 -0.00163400 -0.50988300
C 2.24183800 1.36578800 0.35252600
C 3.34183900 0.55530200 0.51794600
C -0.53041300 -0.03860400 -0.25621600
C -1.21830200 -1.19213800 0.12583600
C -1.21856000 1.16903200 -0.37933200
C -2.58157000 -1.12840700 0.37570100
C -2.57823500 1.22154900 -0.11269600
C -3.26819400 0.07469000 0.26337300
H 2.17450300 2.03239700 -0.49736000
H 4.15149400 0.58545600 -0.20108000
H -0.68494600 -2.13110700 0.21584400
H -0.67739000 2.05606800 -0.68662400
H -3.10958300 -2.02989600 0.66524100
H -3.10332900 2.16511500 -0.20779400
H -4.33199200 0.11739900 0.46389700
H 3.58410600 0.15579100 1.49450500
H 1.59514200 1.59836700 1.19110000
N 2.64135900 -1.32951600 -0.16442000
N 1.54571000 -1.05640200 -0.43434800
N 0.85172700 -0.00163400 -0.50988300
C 2.24183800 1.36578800 0.35252600
C 3.34183900 0.55530200 0.51794600
C -0.53041300 -0.03860400 -0.25621600
C -1.21830200 -1.19213800 0.12583600
C -1.21856000 1.16903200 -0.37933200
C -2.58157000 -1.12840700 0.37570100
C -2.57823500 1.22154900 -0.11269600
C -3.26819400 0.07469000 0.26337300
H 2.17450300 2.03239700 -0.49736000
H 4.15149400 0.58545600 -0.20108000
H -0.68494600 -2.13110700 0.21584400
H -0.67739000 2.05606800 -0.68662400
H -3.10958300 -2.02989600 0.66524100
H -3.10332900 2.16511500 -0.20779400
H -4.33199200 0.11739900 0.46389700
H 3.58410600 0.15579100 1.49450500
H 1.59514200 1.59836700 1.19110000

CA-5
E = -474.416074518 a.u.

N 2.86233000 -0.96315300 0.11918400
N 1.64362300 -1.15589600 0.03181600
N 0.93595000 -0.00412200 -0.13706900
C 1.79020000 1.16563000 0.01639000
C 3.15974000 0.48259100 -0.00793000
C -0.45886900 -0.01006300 -0.06286400
C -1.17131900 -1.21436800 -0.05469600
C -1.15307100 1.20029600 -0.01634900
C -2.55438100 -1.19208600 0.00432900
C -2.54180500 1.20255100 0.04027900
C -3.25188800 0.01168000 0.05174300
H 1.64559200 1.86846600 -0.80563200
H 3.69022200 0.62766600 -0.95251900
H -0.62985500 -2.14960000 -0.09009100
H -0.61692800 2.14135100 -0.02656000
H -3.09516300 -2.13179500 0.01249000
H -3.06699100 2.15036400 0.07601300
H -4.33423900 0.01774400 0.09630300
H 3.82150000 0.78287800 0.80386100
H 1.58089900 1.67773800 0.96320800

ωB97XD/6-311G(d,p) gas phase computed total energies, single imaginary frequency, and cartesian coordinates of the stationary points involved in the 32CA reactions of substituted phenyl azides **42** and **43**.

42
E = -600.275927934 a.u.

N -4.35449800 -0.91820600 0.00047100
N -3.52634400 -0.15902000 0.00031800
N -2.72296300 0.77621200 0.00020100
C -0.46809300 1.53107900 -0.00010000
C 0.89551500 1.30937400 -0.00021200
C 1.36464300 0.00305600 -0.00012700
C 0.50404400 -1.08254500 0.00006800
C -0.86195100 -0.85814400 0.00018100
C -1.35159800 0.45003000 0.00009500
H -0.86966400 2.53616800 -0.00016200
H 1.60106100 2.12876600 -0.00036400
H 0.90894600 -2.08510800 0.00013000
H -1.54078200 -1.70332400 0.00033400
N 2.81588200 -0.23600700 -0.00024900
O 3.54455200 0.73542600 -0.00040200
O 3.19551600 -1.38973200 -0.00016800

26
E = -193.096926802 a.u.

C -0.60950400 0.34896800 -0.03107800
C -1.86592400 -0.07110400 0.03346300
C 1.71316400 0.10901100 0.03906900
H 1.87149400 0.83351500 -0.76881500
H -2.09988800 -1.12725400 0.08269500
H 1.84308100 0.60972500 1.00545100
H -2.67399500 0.64678400 0.02975400
H 2.45003700 -0.68753300 -0.05048200
H -0.35825900 1.40829000 -0.08023500
O 0.44263900 -0.50059700 -0.05838600

TS-42-o
E = -793.342493257 a .u.
Freq = -468.52i cm^{-1}

N -3.04659800 -1.05655500 -1.00596300
N -1.90961100 -0.84893800 -1.13841300
N -1.17375900 0.18393000 -1.01800000
C -3.68976800 0.71435000 0.03116200
C -2.59928600 1.52729200 -0.18522400
C -5.00259100 -0.64601800 1.40175800
H -5.92667300 -0.11083000 1.15119000
H -1.96195500 1.78695700 0.65076600
H -4.90597800 -1.52667900 0.76072000

C 0.89040800 1.24156600 -0.50613000
C 2.21957300 1.20478900 -0.13215300
C 2.82947900 -0.02511500 0.07004000
C 2.13608200 -1.21543400 -0.09159100
C 0.80283700 -1.17820300 -0.45469200
C 0.16880600 0.05268700 -0.66423000
H 0.39662900 2.18859000 -0.68385100
H 2.79376900 2.11175600 -0.00210200
H 2.64625500 -2.15465800 0.07303700
H 0.24693900 -2.09803900 -0.58432000
H -2.59218800 2.17588600 -1.04858400
H -5.04080100 -0.95422400 2.44497800
H -4.56247100 0.76915000 -0.61392100
O -3.87625700 0.20151700 1.27204000
N 4.24366300 -0.06734900 0.46060400
O 4.82182000 0.99275800 0.59888800
O 4.75160900 -1.15940100 0.62292800

TS-42-m
E = -793.352478400 a.u.
Freq = -362.70i cm^{-1}

N 3.10552900 -2.02491700 0.05749200
N 1.99676800 -1.65033300 0.02313700
N 1.45401600 -0.53325500 -0.28762600
C 3.53792900 0.62400000 -0.43007300
C 4.27541900 -0.53883200 -0.51471200
C 2.55684000 2.33188100 0.81734700
H 2.54735400 2.97324600 -0.07014200
H 5.00429200 -0.72618600 0.26307600
H 1.57411100 1.87237900 0.95447000
C -0.49863700 0.77061800 -0.65776200
C -1.86183000 0.97791700 -0.58409900
C -2.66727300 -0.01500000 -0.04405100
C -2.13029000 -1.20888600 0.41758800
C -0.76590700 -1.41304100 0.34609500
C 0.07062300 -0.42266300 -0.19073100
H 0.14502400 1.52608900 -1.09160600
H -2.31317600 1.89271700 -0.94293100
H -2.78783800 -1.96185600 0.83049300
H -0.33416200 -2.33819800 0.70587200
H 4.49356600 -0.92231900 -1.50251800
H 2.81987600 2.92251000 1.69177900
H 3.07213900 1.08397500 -1.29491600
O 3.54228900 1.31704700 0.69963500
N -4.11400700 0.20094000 0.03683600
O -4.55094000 1.26033300 -0.37094400
O -4.79367100 -0.69055000 0.50755000

CA-42-o
E = -793.425013371 a.u.

N 3.13824500 1.16979800 -0.38536800
N 1.91417100 1.31535100 -0.27695300
N 1.23925600 0.13477300 -0.31153400

C 3.48791000 -0.27545800 -0.44879800
C 2.13939600 -0.99193200 -0.47662100
C 5.50178500 -0.12297100 0.75310000
H 6.09173800 -0.42951100 -0.12091900
H 2.07197800 -1.69263500 0.35799600
H 5.48361500 0.96844500 0.81001900
C -0.79549700 -1.14369300 -0.21195600
C -2.17276700 -1.20223800 -0.09162500
C -2.88990900 -0.02715900 0.05516500
C -2.25553400 1.20845900 0.08513000
C -0.88270100 1.27253600 -0.03412700
C -0.13943600 0.09248100 -0.18472200
H -0.23358900 -2.06169900 -0.32478000
H -2.69607300 -2.14828000 -0.11002600
H -2.84727200 2.10607200 0.20208700
H -0.37052700 2.22375000 -0.01223200
H 1.95022600 -1.50995500 -1.41952500
H 5.95723200 -0.53035800 1.65409700
H 4.08827100 -0.43293100 -1.35381300
O 4.19111600 -0.65790600 0.68670100
N -4.34968900 -0.08905000 0.18211500
O -4.94919000 0.96025100 0.31077900
O -4.87304600 -1.18599000 0.15076900

CA-42-m
E = -793.425074370 a.u.

N 3.44095800 -1.71659100 -0.09233500
N 2.23086400 -1.69990200 0.14460700
N 1.66000000 -0.48197500 -0.17232200
C 2.69184800 0.51203200 -0.43523400
C 3.86374900 -0.42960400 -0.66948100
C 2.08313400 2.33123600 0.98284000
H 1.86609500 2.95430400 0.10455500
H 4.76145300 -0.06806300 -0.17109500
H 1.14579400 1.92763700 1.37827700
C -0.34167900 0.78677300 -0.68002200
C -1.71718200 0.92032500 -0.64268000
C -2.47906400 -0.07648700 -0.05548600
C -1.88818600 -1.20702900 0.49072700
C -0.51418800 -1.34099600 0.45864600
C 0.27631800 -0.34065300 -0.12475600
H 0.24781000 1.56324900 -1.14835200
H -2.20745100 1.78528800 -1.06790000
H -2.51133700 -1.96770100 0.94092000
H -0.03729700 -2.21465100 0.87866600
H 4.07686000 -0.59783000 -1.72789900
H 2.55434700 2.94966300 1.74524800
H 2.42786100 1.12616300 -1.30301200
O 3.00598800 1.30925900 0.66714800
N -3.93787000 0.06666400 -0.01425600
O -4.41909900 1.07476600 -0.49441100
O -4.57817700 -0.83015100 0.49768900

43
E = -510.302839447 a.u.

N 4.20943300 -0.67332500 -0.00083900
N 3.31782100 0.01652600 -0.00037900
N 2.43443300 0.86777800 -0.00022200
C 0.10247900 1.38921900 0.00013800
C -1.24222100 1.03905600 0.00028600
C -1.61066600 -0.30501000 0.00020200
C -0.61762600 -1.28602400 -0.00002800
C 0.71865000 -0.93371600 -0.00017500
C 1.08815800 0.41284000 -0.00009100
H 0.39733700 2.43141400 0.00020300
H -1.98615500 1.82443500 0.00046500
H -0.91895300 -2.32624000 -0.00009000
H 1.47332100 -1.71310800 -0.00035000
C -3.92911000 0.19567200 0.00056000
H -4.85691900 -0.37332000 0.00062900
H -3.89477300 0.82854700 0.89495800
H -3.89501100 0.82871600 -0.89372800
O -2.88858000 -0.75619000 0.00033100

40
E = -170.808642745 a.u.

C 1.59595100 -0.36043000 0.00000000
H 1.42553700 -1.43042000 0.00000000
H 2.62146800 -0.01214600 0.00000000
C 0.58817200 0.50672600 0.00000000
C -0.78212100 0.09417500 0.00000000
N -1.88824500 -0.22539300 0.00000000
H 0.75869900 1.57749200 0.00000000

TS-43-o
E = -681.085043861 a.u.
Freq = -506.59i cm^{-1}

C -2.31405800 -0.80876400 -1.23094500
H -2.25464600 -1.83822300 -1.55832700
H -1.62987800 -0.11771900 -1.70975600
C -3.51849300 -0.33937300 -0.72530200
H -4.36782100 -1.00080600 -0.61591900
C -3.80129100 1.06000400 -0.72812800
N -4.01126900 2.19363000 -0.72923800
C 0.16950600 -0.58317100 0.34829700
C 1.12722800 -1.34419800 -0.30318100
C 0.51608800 0.66542000 0.87239200
N -1.15900100 -1.08442200 0.37312300
C 2.42991500 -0.87702100 -0.43983800
C 1.81147700 1.12428900 0.75939600
N -1.93588200 -0.72755900 1.31154300
C 2.77940700 0.35991800 0.09842900
N -3.04617600 -0.45062400 1.45850000
H 0.85058100 -2.31274100 -0.70255800

H -0.23218300 1.27244800 1.36987100
H 3.15716900 -1.49016900 -0.95456200
H 2.10260800 2.08430600 1.16692100
O 4.01374200 0.90472400 0.03531600
C 5.03281100 0.18007600 -0.62050700
H 4.78811900 0.01076200 -1.67516700
H 5.92755200 0.79573100 -0.55470000
H 5.21932000 -0.78164200 -0.12948600

TS-43-m
E = -681.084045435 a.u.
Freq = -488.21i cm^{-1}

C 3.89256200 0.38257200 -0.25817200
H 4.02749000 0.79194600 -1.25059600
H 4.77831400 -0.02392300 0.21401100
C 2.87286900 0.86666900 0.55044200
C 0.15757700 -0.68291100 0.38271100
C -0.57794000 -0.48372300 1.55144000
C -0.47390800 -0.58462100 -0.85151000
N 1.54929800 -0.87926600 0.52481300
C -1.92472200 -0.19587500 1.48361400
C -1.83309600 -0.31483600 -0.92629800
N 2.19774700 -1.49126800 -0.36965600
C -2.56505900 -0.11227200 0.24364600
N 3.22791200 -1.38875800 -0.90568400
H -0.07569600 -0.55629700 2.50864500
H 0.09640800 -0.72004100 -1.76351600
H -2.51142000 -0.03392300 2.37903800
H -2.30138400 -0.24918500 -1.89882900
C 1.93779900 1.81783500 0.03794900
N 1.17014500 2.56455400 -0.38813300
H 2.93974900 0.80475600 1.62772700
O -3.88614400 0.16637900 0.28229400
C -4.57795200 0.30459300 -0.94097500
H -4.55927400 -0.62622500 -1.51909300
H -5.60681300 0.54148900 -0.67739600
H -4.16271700 1.11895100 -1.54480900

CA-43-o
E = -681.151080422 a.u.

C 2.04296200 -0.80310600 -0.49299900
H 1.85630100 -1.34178200 -1.42166000
H 1.92849000 -1.48604200 0.35656700
C 3.39654500 -0.07906200 -0.49019700
H 3.79257300 0.04428800 -1.50299600
C 4.41514700 -0.72528000 0.32864400
N 5.20159900 -1.26395000 0.96977300
C -0.23047100 0.28322100 -0.18960400
C -0.88712300 -0.93314900 -0.30657300
C -0.97377600 1.44002800 0.07210900
N 1.16573000 0.35125700 -0.36029800
C -2.27202200 -1.01064500 -0.16129200

C -2.34139400 1.36073800 0.22029600
N 1.85101500 1.44030200 0.04049900
C -3.00785900 0.13657600 0.10487400
N 3.08213800 1.29383600 0.02007000
H -0.33617200 -1.84264300 -0.51314900
H -0.46698000 2.39089900 0.16428000
H -2.75072300 -1.97580400 -0.25826400
H -2.92690000 2.24810100 0.42714300
O -4.35287000 0.17713600 0.26587800
C -5.06811400 -1.03368800 0.16517700
H -4.74935700 -1.75312400 0.92859000
H -6.11400500 -0.78013700 0.32746400
H -4.95700900 -1.48476100 -0.82792200

CA-43-m
E = -681.150549391 a.u.

C 3.71402200 -0.53133100 0.45301000
H 4.50370700 -0.16727600 -0.20357900
H 4.14121400 -0.72980700 1.43673200
C 2.49791000 0.42233300 0.51940400
C 0.06793900 -0.23590600 0.07466600
C -0.41925200 1.01387200 0.46177200
C -0.83175900 -1.22942800 -0.29745900
N 1.45400800 -0.48343400 0.06491900
C -1.78107800 1.25651800 0.47871800
C -2.19829600 -0.98225500 -0.28136700
N 1.95306800 -1.70158200 -0.25985300
C -2.68531100 0.26362700 0.10883000
N 3.17387700 -1.79327400 -0.08792800
H 0.25402300 1.81630400 0.73762900
H -0.46091300 -2.19915100 -0.59944000
H -2.16538000 2.22490400 0.77366300
H -2.86932400 -1.77762500 -0.57732300
C 2.64503000 1.59831300 -0.35072300
N 2.78224700 2.52461300 -1.01705500
H 2.29698700 0.77532000 1.53559900
O -3.99756500 0.60170000 0.15938100
C -4.94710800 -0.36857600 -0.22149200
H -4.90285300 -1.25158100 0.42683800
H -5.92105700 0.10513500 -0.11333200
H -4.81086400 -0.67708900 -1.26457100