On the Mechanism of the Copper-Mediated C–S Bond Formation in the Intramolecular Disproportionation of Imine Disulfides

Supporting Information

Tibor András Rokob, Lubomír Rulíšek,* Jiří Šrogl, Ágnes Révész, Emilie L. Zins, and Detlef Schröder*

Institute of Organic Chemistry and Biochemistry, Flemingovo nám. 2, 16610 Prague 6, Czech Republic

Contents

1. Alternative routes from A to the products

Potential energy profile for some alternative routes, actually starting from the copper(III) disulfide intermediate (**B**), is shown in Figure S1. On one of these routes, the copper-nitrogen dative bond is broken first via $\mathbf{TS_{BB_T}}$, leading to the copper(III) complex $\mathbf{B_T}$ (Figure S2). No detailed analysis was done for the electronic structure of $\mathbf{B_T}$ is , but it was found to be a closed-shell singlet, with the triplet being 11.4 kcal mol^{-1} higher in energy; the copper seems here to be capable of mediating a strong antiferromagnetic interaction. The *d* orbital population is 9.56.

Passing $\mathbf{TS_{B_TD_S}}$, C–S bond formation can lead to an analogue of the heterocyclic copper(III) intermediate **D**, termed here $\mathbf{D_S}$, where the heterocyclic ring is attached to the copper via the sulfur atom (Figure S3). As it may be expected from the difficulty to draw favorable resonance forms for $\mathbf{D_S}$, it is significantly less stable than **D** (the energy difference amounts to 17.3 kcal mol^{-1}). Analysis of the electronic structure of $\mathbf{D_S}$ shows radical sites mostly localized on the *nitrogen* of the heterocyclic ring, and on the sulfur atom of the other ligand. The singlet is by 0.06 kcal mol^{-1} more stable than the triplet.

Like **D**, $\mathbf{D_S}$ can yield an **E**-type isomer via hydrogen transfer. The transition structure was only located for the transfer to the sulfur atom; relaxed PES scans showed markedly higher energy for the other two pathways. This transition structure ($\mathbf{TS_{D_SE_{SS}}}$, Figure S4) is the highest point along the whole route (37.4 kcal mol^{-1}). In the resulting isomer $\mathbf{E_{SS}}$, the 2-phenylbenzothiazole moiety is coordinated via its sulfur atom to the copper, which seems to be a destabilizing factor: $\mathbf{E_{SS}}$ is less stable than the corresponding $\mathbf{E_S}$ by 14.4 kcal mol^{-1}.

Somewhat unexpectedly, hydrogen transfer can directly proceed from isomer **B**. In transition structure $\mathbf{TS_{BE_{SS}}}$, shown in Figure S5, the future benzothiazole is formed in its zwitterionic open form (see the bracketed structure on Figure S1); this is confirmed by the C≡N bond length showing partial triple bond character. Despite the expected instability of this open form, the transition structure lies only at 34.7 kcal mol^{-1}; on the other hand, the subsequent closure of the thiazole ring by C–S bond formation is a spontaneous process with no associated barrier.

As an alternative possibility, we searched for S–S bond cleavage concerted with hydrogen transfer from C to S, and perhaps even with C–S bond formation, which would circumvent the high valent copper species. However, no such multiply-centered transition structure could be found computationally. Apparently, the energy necessary for the concerted process is so high that simple homolytic S–S bond breaking can compete, even in the absence of the copper at an appropriate position to catalyze it. During the exploration of this region of the PES, we were only able to identify local

minima **I** and **II** corresponding to diradicaloid intermediates; not only are these quite high in energy (46.5 kcal mol^{-1} and 39.8 kcal mol^{-1} higher than **A**) but they also convert into copper(III) structures, if subjected to relaxed PES scans toward H-atom abstraction.

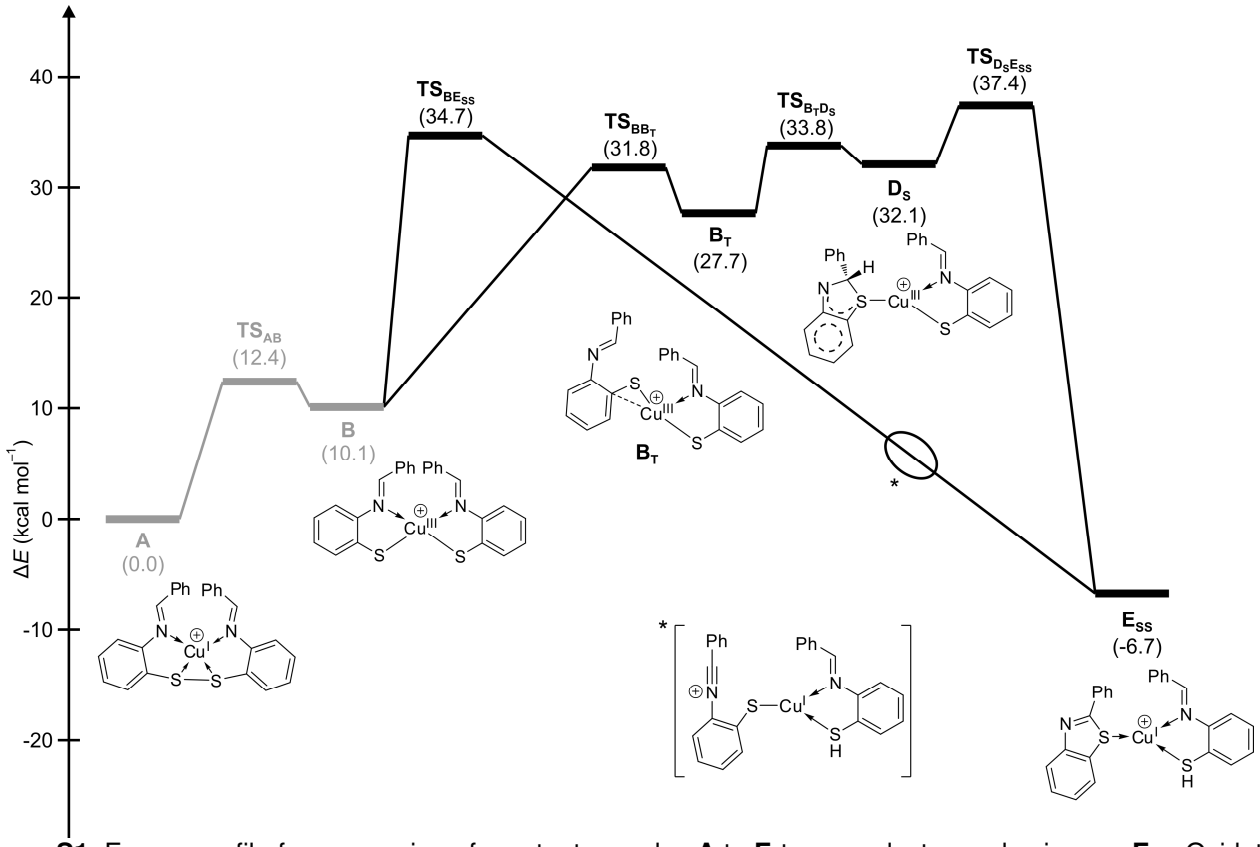

Figure S1. Energy profile for conversion of reactant complex **A** to **E**-type product complex isomer $\mathbf{E_{SS}}$. Oxidative addition in **A** yielding **B** is discussed in the main text and shown in gray here. The structure marked with asterisk and shown in brackets cannot be identified as a stationary point on the route, but analysis of the geometry of $\mathbf{TS_{BE_{SS}}}$ and its decay towards the product $\mathbf{E_{SS}}$ points to its involvement (see also text).

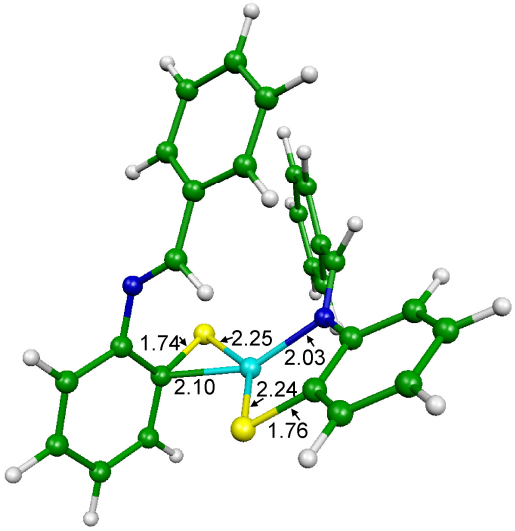

Figure S2. Optimized structure of $\mathbf{B_T}$

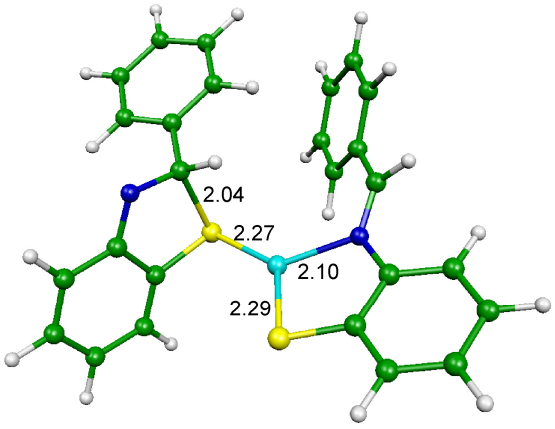

Figure S3. Optimized structure of $\mathbf{D_S}$

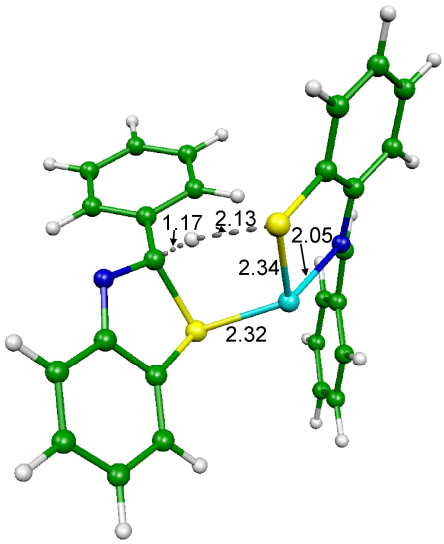

Figure S4. Optimized structure of $\mathbf{TS_{D_SE_{SS}}}$

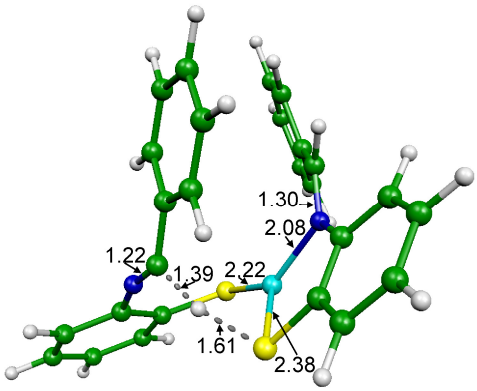

Figure S5. Optimized structure of $\mathbf{TS_{BE_{SS}}}$

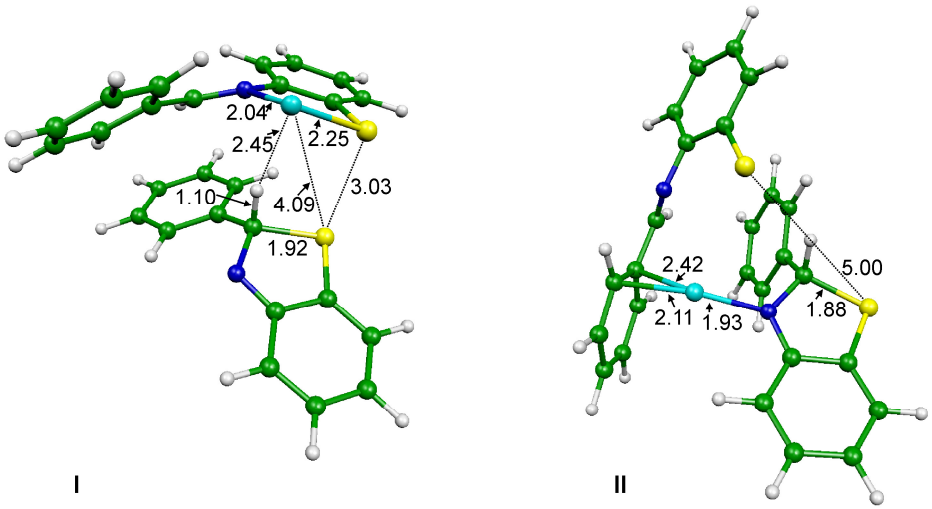

Figure S6. Optimized structure of diradicaloid minima **I** and **II**

2. Comparison of experimental IRMPD for *m/z* 487 with computations

Computed intensities were subject to an arbitrary overall scaling separately in each graph.

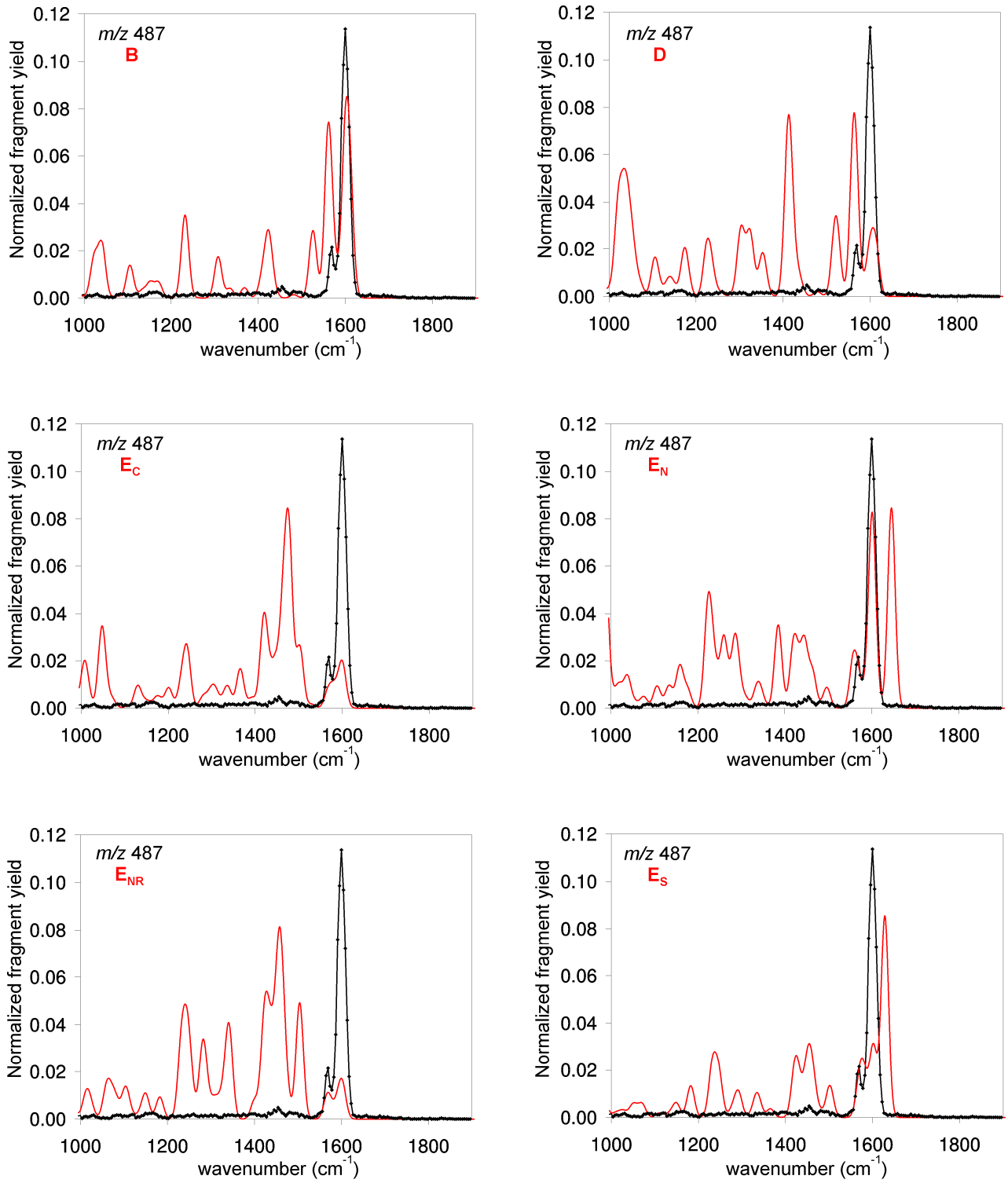

Figure S7. Matching of various calculated IR spectra with experimental IRMPD spectrum of *m/z* 487

3. Comparison of experimental IRMPD for *m/z* 294 with computations

Computed intensities were subject to an arbitrary overall scaling separately in each figure.

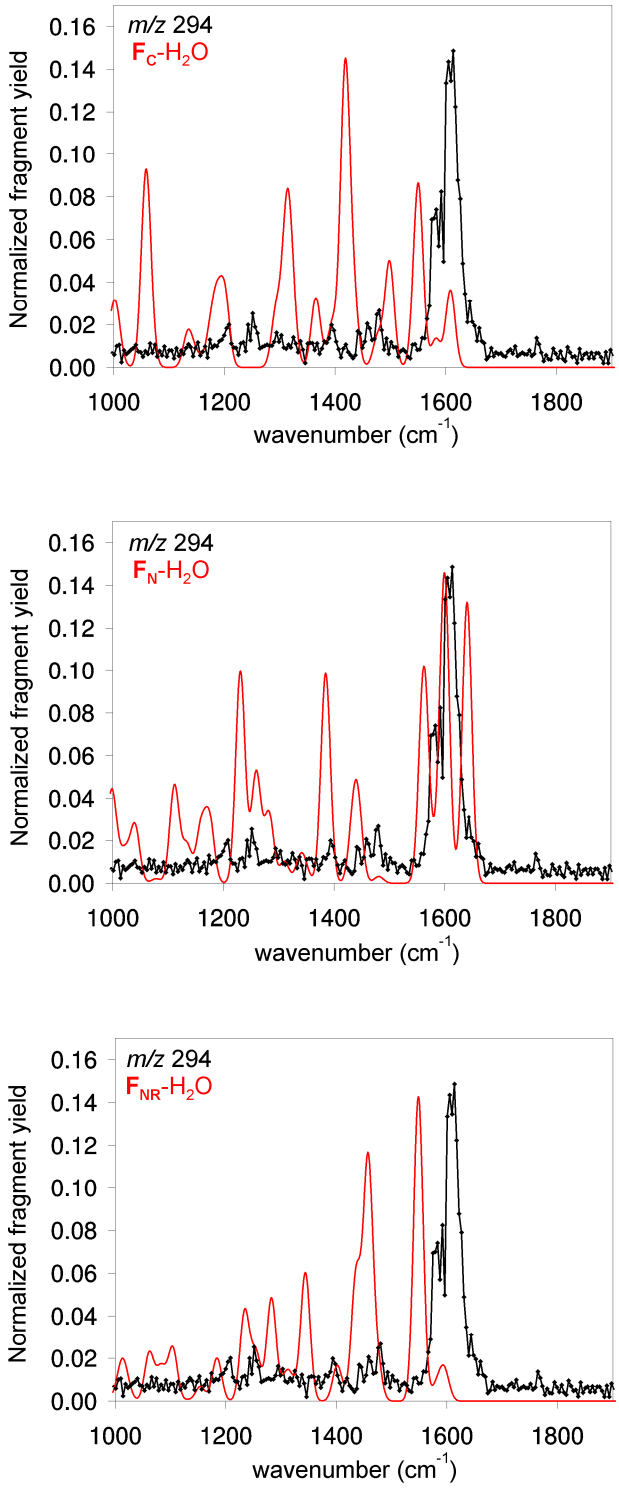

Figure S8. Matching of various calculated IR spectra with experimental IRMPD spectrum of *m/z* 294

4. Energy profile for CuH loss

In Figure S9, a detailed energy profile for CuH loss from $\mathbf{F_S}$ is shown. The process starts with an intramolecular proton transfer to form the somewhat less stable **F**-type isomer $\mathbf{F_N}$. Carbon-sulfur bond formation can produce the ring-closed isomer $\mathbf{F_{NR2}}$, and a minor change in copper coordination can yield $\mathbf{F_{NR3}}$.

At the B3LYP-D/def2-SVP level, which was used for geometry optimization, $\mathbf{TS_{F_NF_{NR2}}}$ is a true transition structure, and $\mathbf{F_{NR2}}$ is somewhat lower in energy than that TS. Subsequent single-point B3LYP-D/def2-TZVPP calculations predict $\mathbf{F_{NR2}}$ to be higher; considering the PES up to $\mathbf{F_{NR3}}$ it seems that the fine details of copper coordination to the closed form may slightly differ using the two basis sets, but the key conclusion, i.e., existence of a closed-ring isomer with the copper and the hydrogen to be eliminated in *cis* position, is valid regardless of the method.

The highest point on this route corresponds to the copper-hydrogen bond formation via $\mathbf{TS_{F_{NR3}G}}$ (Figure S10). In the resulting isomer **G**, copper is still complexed, but only by aromatic π-electrons; copper(I) hydride can directly dissociate to form **2**-H^+ with *m/z* 212.

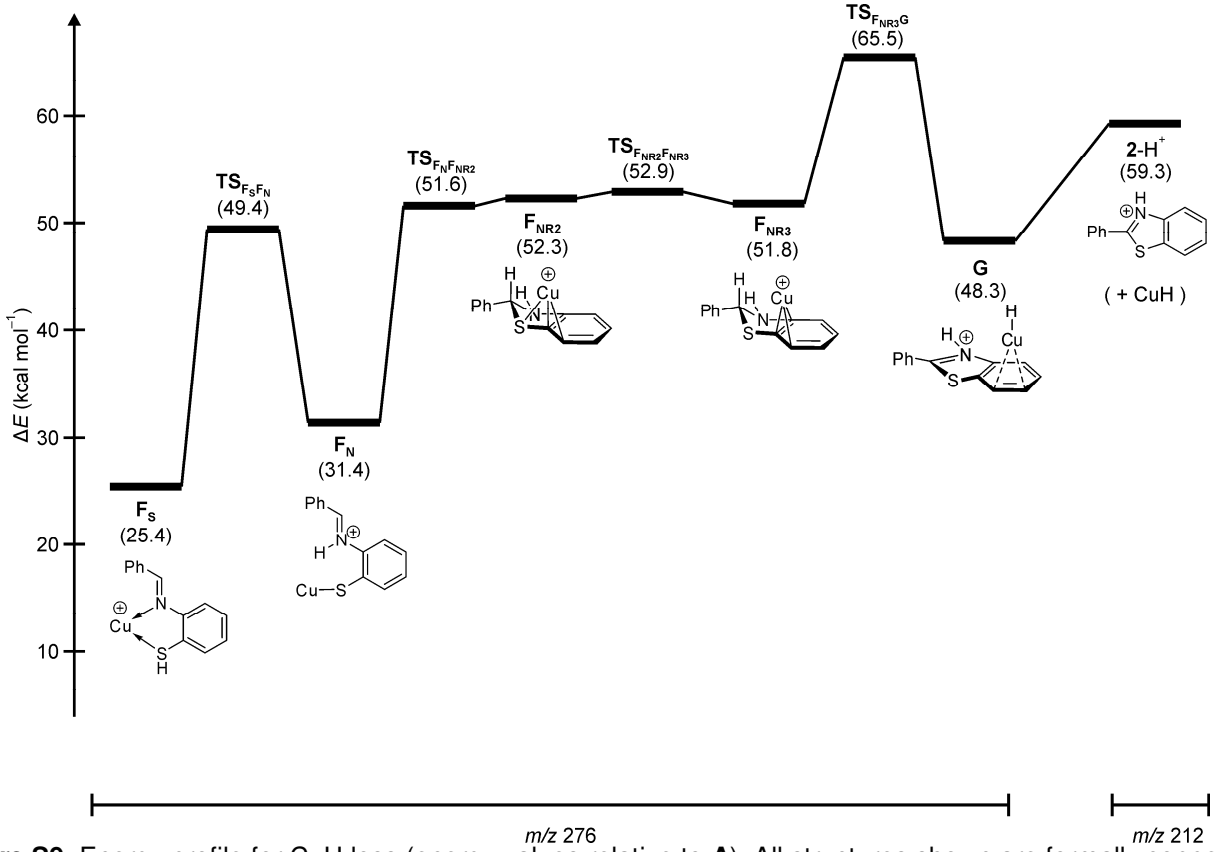

Figure S9. Energy profile for CuH loss (energy values relative to **A**). All structures shown are formally copper(I) species, and have closed-shell singlet electronic ground states.

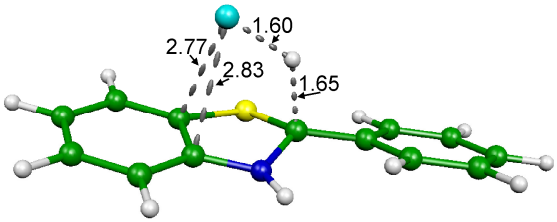

Figure S10. Transition structure $\mathbf{TS_{F_{NR3}G}}$

5. Experimental breakdown curve for CuH loss

Experimentally, upon collision-induced dissociation of the ion with *m/z* 276, the only fragment ion observed is *m/z* 212 concomitant with loss of neutral CuH. Energy-resolved CID measurements lead to an apparent threshold of (56 ± 6) kcal mol^{-1} for the CuH loss from *m/z* 276 (Figure S11). Once again, the experimental appearance energy is somewhat higher than the computed value of 40.1 kcal mol^{-1}, similarly to the case of fragmentation of **1**/Cu^+. However, also this fragmentation does not correspond to a simple bond cleavage, but rather involves a complex rearrangement, such that an overestimation of the experimental threshold is indeed expected.

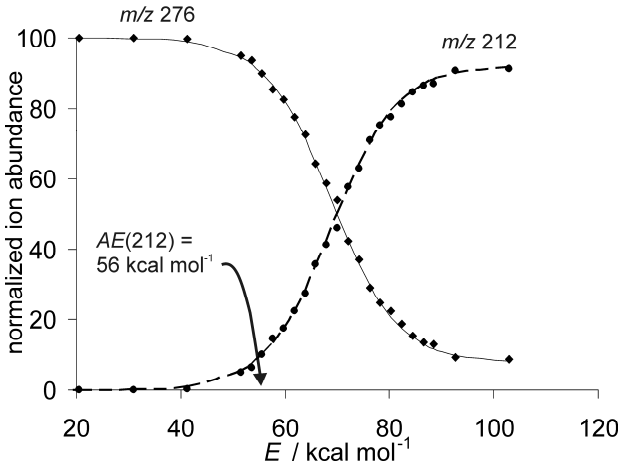

Figure S11. CID breakdown diagram of *m/z* 276 to afford fragment with *m/z* 212

6. M06 and spin-projected results, imaginary frequencies, $\langle S^2 \rangle$ values

Table S1. Imaginary frequencies of transition states (in cm^{-1}), $\langle S^2 \rangle$ values, and comparison of B3LYP, spin-projected B3LYP and M06 energetics (in kcal mol^{-1}) for the copper based reaction mechanism. Zero-point vibrational energies are included, with the exception of singlet-triplet gaps. Structure symbols with primes (e.g. **D'**, **D''**) refer to less stable conformers of the same compound. For each transition state, the structures connected by it are given in parentheses. Turquoise numbers are relative to **A**, with the appropriate inclusion of the lost fragments (**2**, CuH) if necessary. Dark red numbers are relative to closed **3**, green numbers to **1**, black numbers to the respective singlet states. (T) refers to single point triplet calculations, while (SP-S) denotes single point spin-projected energies. The latter were calculated only for B3LYP using $\langle S^2 \rangle$ values in the table for the broken symmetry states, and $\langle S^2 \rangle$=2 for the triplet states.

	Imaginary frequency	$\langle S^2 \rangle$ (B3LYP)	ΔE (B3LYP) incl. 0.97ZPVE	$\langle S^2 \rangle$ (M06)	ΔE (M06) incl. 0.97ZPVE
half-**1** (S-S homolytically cleaved)		0.7681	**48.02**	0.7725	**51.54**
opened **3** (*E*)		0.0000	**1.04**	0.0000	**4.57**
Cu^+ + **1**		0.0000	**123.76**	0.0000	**122.80**
A		0.0000	**0.00**	0.0000	**0.00**
A'		0.0000	**0.10**	0.0000	**-0.67**
$\mathbf{TS_{A/E,Z\text{-}A}}$ (**A** / *E,Z*-**A'**)	i275.93	0.0000	**22.70**	0.0000	**21.20**
E,Z-**A**		0.0000	**4.00**	0.0000	**4.16**
E,Z-**A'**		0.0000	**6.45**	0.0000	**6.18**
$\mathbf{TS_{AB}}$ (**A** / **B**)	i80.33	0.4137	**12.42**	0.3953	**17.21**
$\mathbf{TS_{AB}}$ (**A** / **B**) (T)		2.0258	**5.41**		
$\mathbf{TS_{AB}}$ (**A** / **B**) (SP-S)			**11.01**		
B		1.0258	**10.14**	1.0337	**16.07**
B (T)		2.0261	**-1.05**		**-1.19**
B (SP-S)			**11.25**		
B'		1.0212	**11.31**	1.0317	**17.83**
$\mathbf{TS_{BC}}$ (**B** / **C**)	i33.37	1.0292	**27.90**	1.0388	**33.21**
$\mathbf{TS_{BC}}$ (**B** / **C**) (T)		2.0329	**0.05**		
$\mathbf{TS_{BC}}$ (**B** / **C**) (SP-S)			**27.85**		
C		1.0274	**26.11**	1.0367	**31.89**
C (T)		2.0291	**0.00**		
C (SP-S)			**26.11**		
$\mathbf{TS_{CD}}$ (**C** / **D**)	i124.10	0.9752	**27.89**	0.9955	**34.47**
$\mathbf{TS_{CD}}$ (**C** / **D**) (T)		2.0233	**0.48**		
$\mathbf{TS_{CD}}$ (**C** / **D**) (SP-S)			**27.43**		
D		0.8764	**14.77**	0.9440	**18.89**
D (T)		2.0317	**1.22**		**0.77**
D (SP-S)			**13.81**		
D'		0.9748	**15.91**	0.9964	**18.70**
D''		0.9810	**16.36**	1.0220	**18.90**
$\mathbf{TS_{AD}}$ (**A'** / **D'**)	i172.21	0.0000	**31.14**	0.0000	**32.09**
$\mathbf{TSDE_S}$ (**D''** / $\mathbf{E_S}$)	i733.82	0.1597	**25.67**	0.2565	**27.69**
$\mathbf{TSDE_S}$ (**D''** / $\mathbf{E_S}$) (T)		2.0280	**9.16**		
$\mathbf{TSDE_S}$ (**D''** / $\mathbf{E_S}$) (SP-S)			**24.87**		
$\mathbf{TSDE_C}$ (**D** / $\mathbf{E_C}$)	i1148.24	0.0011	**33.81**	0.0011	**37.77**
$\mathbf{TSDE_C}$ (**D** / $\mathbf{E_C}$) (T)		2.0205	**12.13**		
$\mathbf{TSDE_C}$ (**D** / $\mathbf{E_C}$) (SP-S)			**33.80**		

TSDE_N (**D'** / **E_N**)	i1056.89	0.2017	**31.60**	0.1714	**36.26**
TSDE_N (**D'** / **E_N**) (T)		2.0215	**10.88**		
TSDE_N (**D'** / **E_N**) (SP-S)			**30.38**		
E_S		0.0000	**-21.07**	0.0000	**-20.77**
E_C		0.0000	**-2.13**	0.0000	**-1.87**
E_N		0.0000	**-21.65**	0.0000	**-21.62**
E_{Cu}		0.0000	**23.87**	0.0000	**28.40**
E_{NR}		0.0000	**-17.24**	0.0000	**-21.09**
TSBB_T (**B'** / **B_T**)	i150.68	0.9041	**31.80**	0.9399	**33.54**
TSBB_T (**B'** / **B_T**) (T)		2.0254	**1.21**		
TSBB_T (**B'** / **B_T**) (SP-S)			**30.80**		
B_T		0.0000	**27.65**	0.0000	**27.71**
B_T (T)			**11.43**		**11.80**
TSB_TD_S (**B_T** / **D_S**)	i122.62	1.0177	**33.77**	1.0378	**35.80**
TSB_TD_S (**B_T** / **D_S**) (T)		2.0403	**0.14**		
TSB_TD_S (**B_T** / **D_S**) (SP-S)			**33.62**		
D_S		1.0346	**32.10**	1.0541	**32.36**
D_S (T)		2.0479	**0.06**		**0.04**
D_S (SP-S)			**32.03**		
TSD_SE_{SS} (**D_S** / **E_{SS}**)	i70.70	0.5373	**37.43**	0.6014	**38.64**
TSD_SE_{SS} (**D_S** / **E_{SS}**) (T)		2.0386	**6.19**		
TSD_SE_{SS} (**D_S** / **E_{SS}**) (SP-S)			**35.16**		
E_{SS}		0.0000	**-6.69**	0.0000	**-9.16**
TSBE_{SS} (**B'** / **E_{SS}**)	i1058.57	0.0000	**34.65**	0.0000	**37.10**
I		0.4673	**46.54**	0.4342	**46.89**
I (T)		2.0314	**8.90**		
I (SP-S)			**43.83**		
II		0.9979	**39.77**	1.0138	**39.80**
II (T)		2.0361	**0.59**		
II (SP-S)			**39.18**		
F_S		0.0000	**25.35**	0.0000	**21.25**
F_S'		0.0000	**25.46**	0.0000	**21.44**
F_C		0.0000	**43.31**	0.0000	**39.10**
F_N		0.0000	**31.44**	0.0000	**28.62**
F_N'		0.0000	**35.31**	0.0000	**32.63**
F_{Cu}		0.8605	**68.64**	0.8522	**70.21**
F_{Cu} (T)		2.0175	**2.91**		
F_{Cu} (SP-S)			**66.44**		
F_{NR}		0.0000	**36.67**	0.0000	**29.92**
TSF_SF_N (**F_S'** / **F_N**)	i138.29	0.0000	**49.39**	0.0000	**46.10**
TSF_NF_{NR2} (**F_N'** / **F_{NR2}**)	i69.03	0.0000	**51.56**	0.0000	**44.57**
F_{NR2}		0.0000	**52.33**	0.0000	**44.17**
TS$F_{NR2}F_{NR3}$ (**F_{NR2}** / **F_{NR3}**)	i31.95	0.0000	**52.88**	0.0000	**44.76**
F_{NR3}		0.0000	**51.78**	0.0000	**44.61**
TS$F_{NR3}G$ (**F_{NR3}** / **G**)	i680.12	0.0000	**65.50**	0.0000	**61.32**
G		0.0000	**48.27**	0.0000	**41.43**
2-H^+		0.0000	**59.30**	0.0000	**53.66**
Cu(half-**1**)$^+$ + half-**1**		0.7654	**77.10**	0.7695	**74.02**

Table S2. Imaginary frequencies of transition states (in cm^{-1}), $\langle S^2 \rangle$ values, and comparison of B3LYP and M06 energetics (in kcal mol^{-1}) for some $ZnCl^+$-containing species. Zero-point vibrational energies are included. Structure symbols with primes (e.g. **D'**, **D''**) refer to less stable conformers of the same compound. For each transition state, the structures connected by it are given in parentheses. Numbers are relative to ZnCl-**A**, with the appropriate inclusion of the lost fragments (**2**) if necessary. Energies of the open shell systems refer to the spin-unprojected broken-symmetry calculations.

	Imaginary frequency	$\langle S^2 \rangle$ **(B3LYP)**	**Δ*E* (B3LYP) incl. 0.97ZPVE**	$\langle S^2 \rangle$ **(M06)**	**Δ*E* (M06) incl. 0.97ZPVE**
$ZnCl^+$		0.0000	**149.44**	0.0000	**147.02**
ZnCl-**B**		1.0311	**29.99**	1.0396	**33.65**
ZnCl-**C**		1.0301	**33.65**	1.0384	**38.77**
ZnCl-**D**		1.0240	**17.42**	1.0353	**18.90**
ZnCl-**D'**		1.0312	**18.61**	1.0401	**19.23**
ZnCl-**D''**		1.0076	**18.64**	1.0256	**19.66**
ZnCl-$\mathbf{TS_{AD}}$ (ZnCl-**A** / ZnCl-**D'**)	i35.19	0.0000	**31.24**	0.0000	**31.22**
ZnCl-$\mathbf{TSDE_S}$ (ZnCl-**D''** / ZnCl-$\mathbf{E_S}$)	i494.47	0.3197	**21.48**	0.3558	**23.24**
ZnCl-$\mathbf{E_S}$		0.0000	**-20.63**	0.0000	**-20.37**
ZnCl-$\mathbf{F_S}$		0.0000	**20.65**	0.0000	**17.44**
Zn(half-**1**)Cl^+ + half-**1**		0.7651	**71.47**	0.7676	**72.36**

7. CID studies of the adducts 1/M$^+$ with other metal ions

In order to probe the ability of other metal ions to mediate the S–S bond cleavage in the title substrate **1**, dilute solutions of this substrate with various metal salts were subjected to ESI, the respective **1**/M$^+$ complexes were mass-selected and probed by CID experiments at variable collision energies under the same conditions as describe for the copper complex in the full text.

7a. Lithium cation Li$^+$

CID of mass-selected **1**/Li$^+$ (*m/z* 431) shows the losses of neutral benzothiazole (Δm = 211), homolytic S–S bond rupture concomitant with loss of a radical (Δm = 212), and expulsion of dihydrobenzothiazole (Δm = 213) to afford ionic fragments at *m/z* 218-220 (Figure S12). All the channels appear at roughly the same appearance energy of 26.8 NCE-%, which corresponds to ca. 55 kcal mol^{-1} (Figure S13).

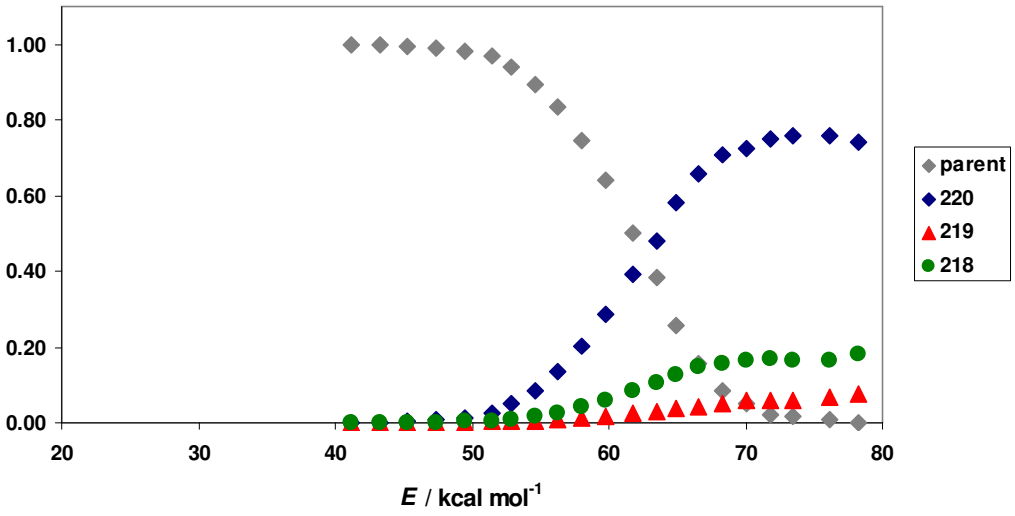

Figure S12. Energy dependent branching ratio upon CID of **1**/Li$^+$.

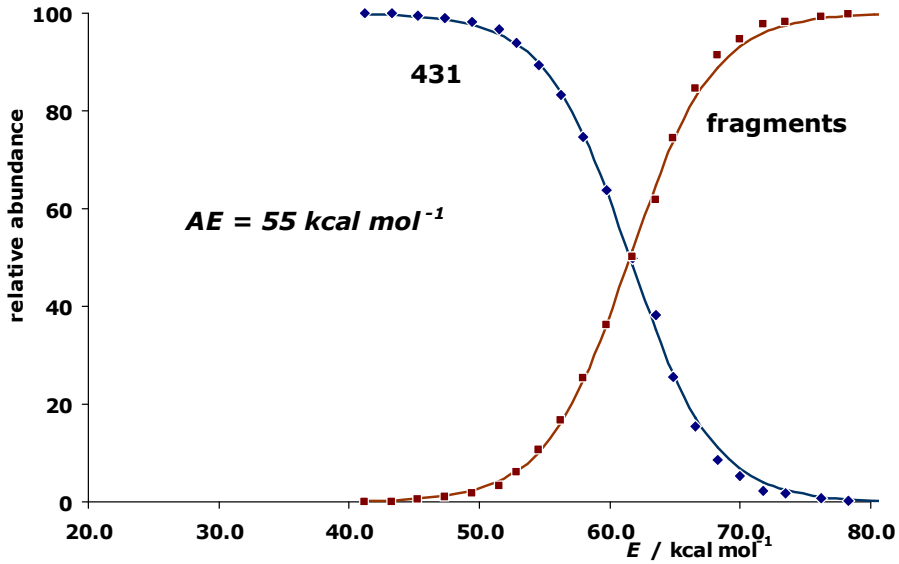

Figure S13. CID breakdown diagram of **1**/Li$^+$ as a function of collision energy.

7b. Sodium cation Na^+

Mass-selected **1**/Na^+ (*m/z* 447) behaves the same way as the Li^+ complex with the radical loss to afford an ionic fragment with *m/z* 235 being even more pronounced (Figure S14). The measured appearance energy of ca. 30.3 NCE-% (Figure S15) is even higher than for Li^+ and corresponds to about 62 kcal mol^{-1}.

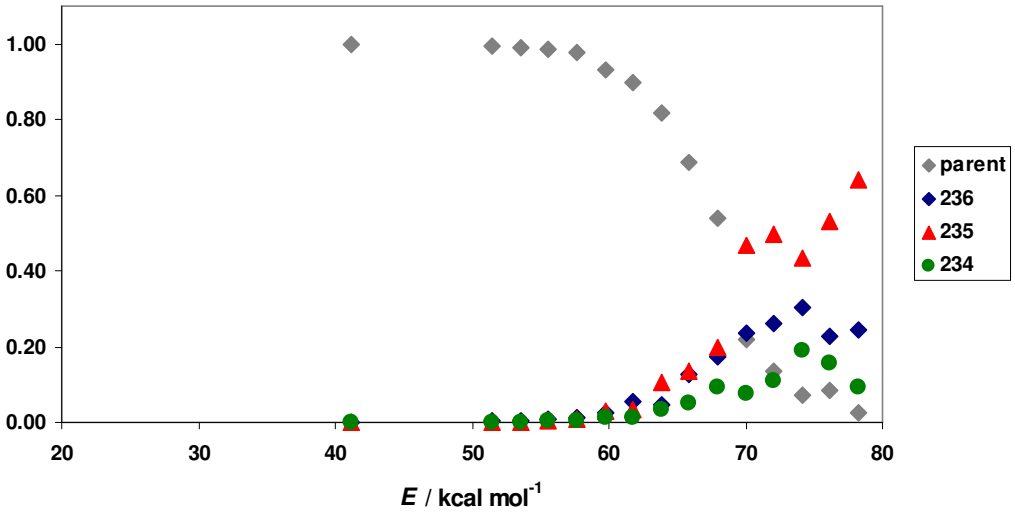

Figure S14. Energy dependent branching ratio upon CID of **1**/Na^+.

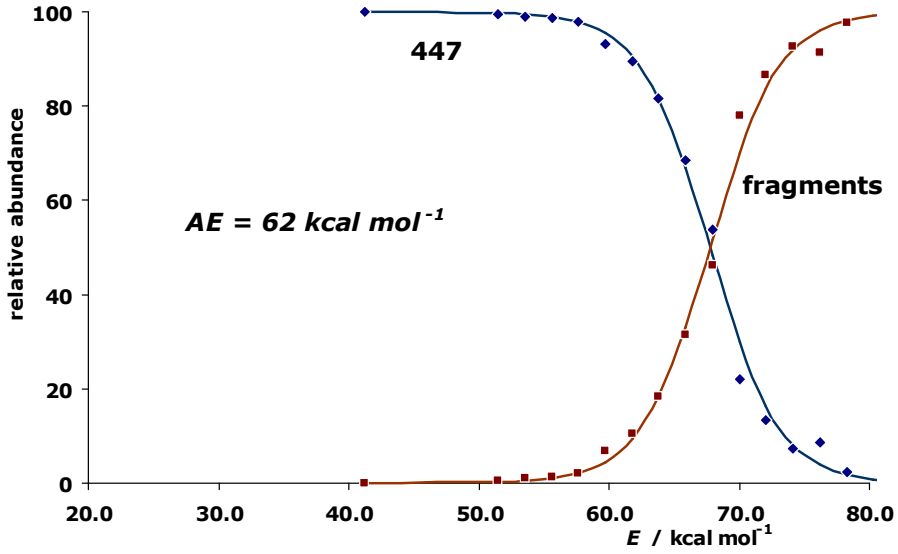

Figure S15. CID breakdown diagram of **1**/Na^+ as a function of collision energy.

7c. Nickel chloride cation $NiCl^+$

CID of mass-selected **1**/$NiCl^+$ (*m/z* 517) shows losses of HCl (ion with *m/z* 481), a combined loss of HCl and benzothiazole (ion with *m/z* 270), and the organic ion **2**/H^+ (*m/z* 212) appearing at elevated CID energies (Figure S16). Loss of neutral benzothiazole without that of HCl (i.e. an ion with *m/z* 306) is negligible. Further, no losses of open-shell fragments are observed. Since the major fragments appear practically at the same energy, the sum of the fragments was modeled (Figure S17), which leads to an appearance energy of 21.0 NCE-% or 43 kcal mol^{-1}.

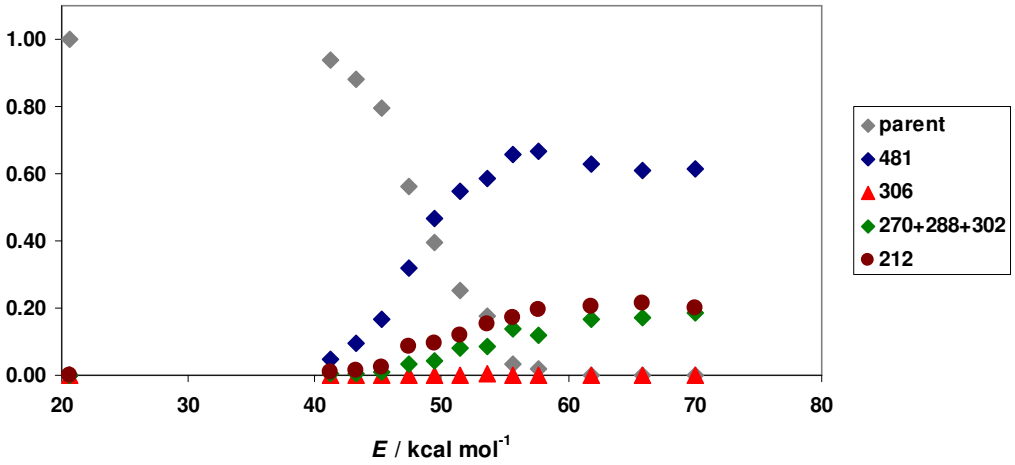

Figure S16. Energy dependent branching ratio upon CID of **1**/$NiCl^+$.

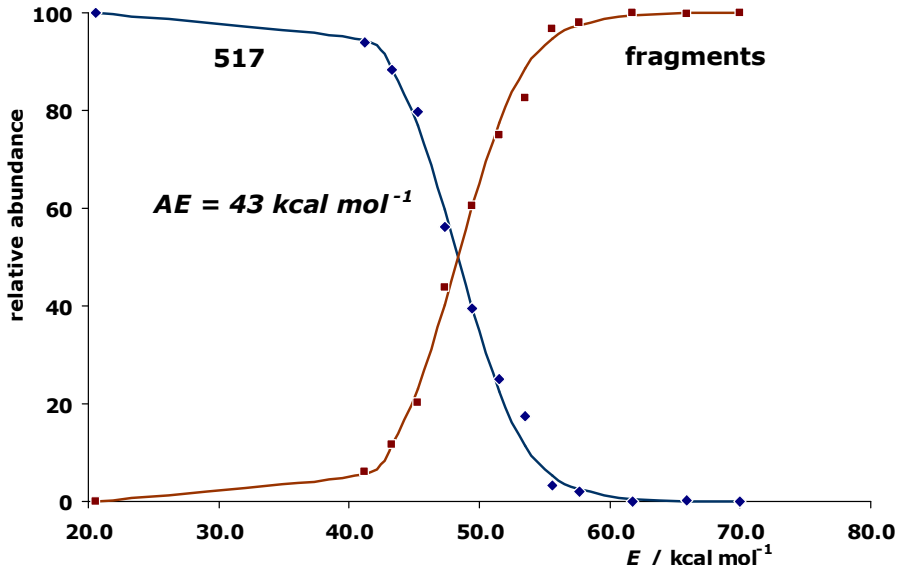

Figure S17. CID breakdown diagram of **1**/$NiCl^+$ as a function of collision energy.

7d. Zinc chloride cation $ZnCl^+$

CID of mass-selected **1**/$ZnCl^+$ (*m/z* 523) shows losses of HCl (ion with *m/z* 487), benzothiazole (ion with *m/z* 312), or both (ion with *m/z* 276) with the organic ion **2**/H^+ (*m/z* 212) appearing at elevated CID energies (Figure S18). No losses of open-shell fragments are observed. Since the three major fragments appear practically at the same energy, the sum of the fragments was modeled (Figure S19), which leads to an appearance energy of 21.8 NCE-% or 45 kcal mol^{-1}.

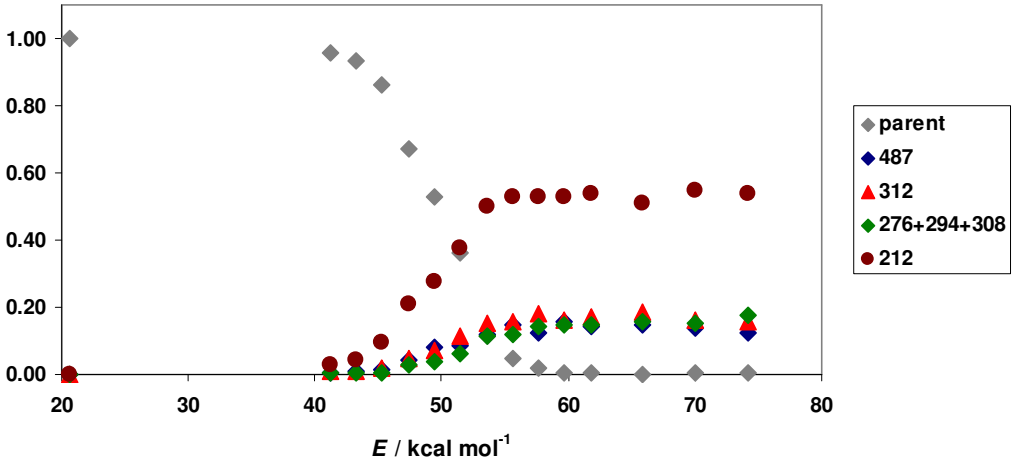

Figure S18. Energy dependent branching ratio upon CID of **1**/$ZnCl^+$.

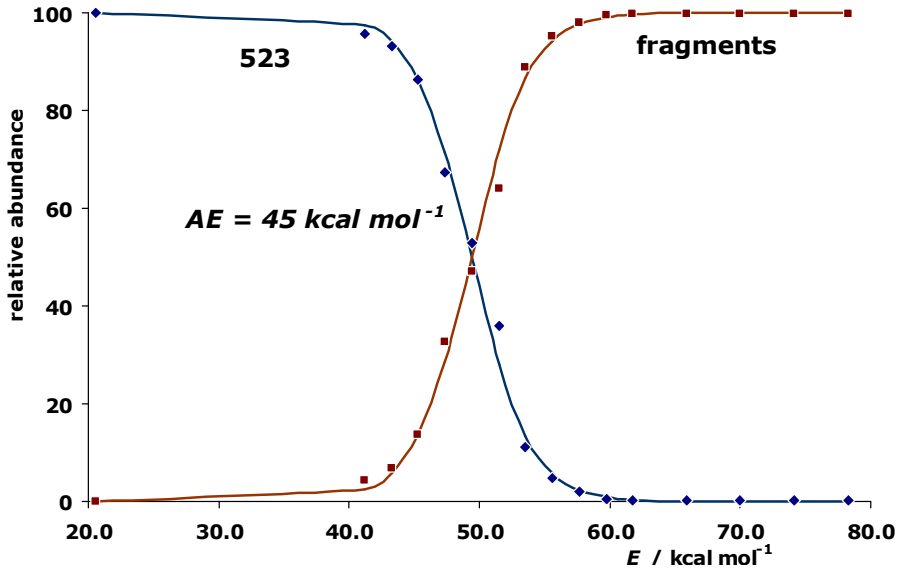

Figure S19. CID breakdown diagram of **1**/$ZnCl^+$ as a function of collision energy.

7e. Silver cation Ag^+

Similarly to copper, mass-selected **1**/Ag^+ (*m/z* 531) loses neutral benzothiazole (resulting in an ionic species at *m/z* 320) as the more or less exclusive fragmentation pathway and this fragment can subsequently lose neutral AgH (Figure S20). The derived appearance energy for the benzothiazole loss channel of 21.1 NCE-% converts to 44 kcal mol^{-1}.

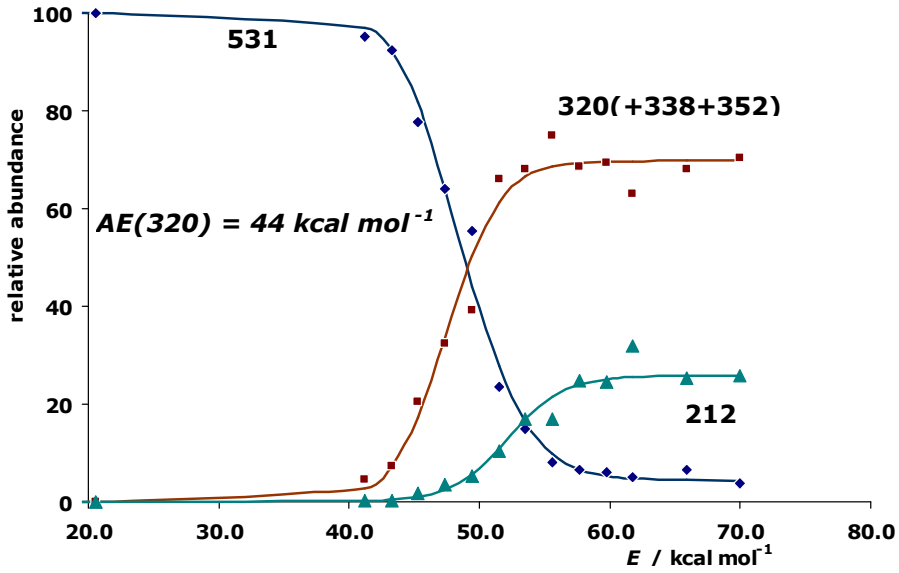

Figure S20. CID breakdown diagram of **1**/Ag^+ as a function of collision energy.

7f. Proton H^+

Last but not least, the CID of protonated **1**/H^+ (*m/z* 425) was examined. Upon CID, **1**/H^+ undergoes competing losses of benzothiazole and its dihydro derivative resulting in fragments at *m/z* 212 and *m/z* 214 (Figure S21). Modeling of the curve yields an appearance energy of 45 kcal mol^{-1}.

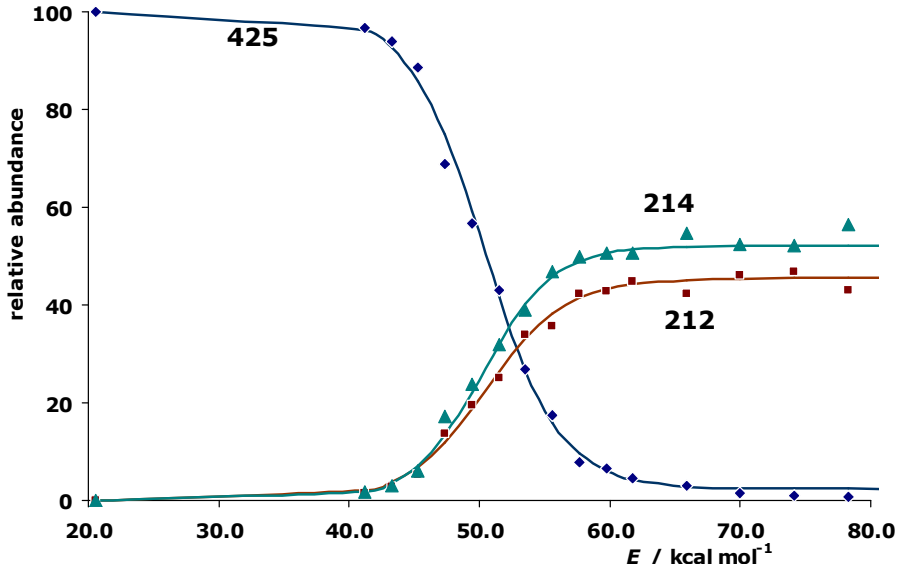

Figure S21. CID breakdown diagram of **1**/H^+ as a function of collision energy.

8. Full references of software packages

Ahlrichs, R.; Armbruster, M. K.; Bachorz, R. A.; Bär, M.; Baron, H.-P.; Bauernschmitt, R.; Bischoff, F. A.; Böcker, S.; Crawford, N.; Deglmann, P.; Sala, F. D.; Diedenhofen, M.; Ehrig, M.; Eichkorn, K.; Elliott, S.; Furche, F.; Glöß, A.; Haase, F.; Häser, M.; Hättig, C.; Hellweg, A.; Höfener, S.; Horn, H.; Huber, C.; Huniar, U.; Kattannek, M.; Klopper, W.; Köhn, A.; Kölmel, C.; Kollwitz, M.; May, K.; Nava, P.; Ochsenfeld, C.; Öhm, H.; Pabst, M.; Patzelt, H.; Rappoport, D.; Rubner, O.; Schäfer, A.; Schneider, U.; Sierka, M.; Tew, D. P.; Treutler, O.; Unterreiner, B.; von Arnim, M.; Weigend, F.; Weis, P.; Weiss, H.; Winter N. *TURBOMOLE 6.2*, University of Karlsruhe, Forschungszentrum Karlsruhe GmbH, TURBOMOLE GmbH, **2010**.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision A.02, Gaussian, Inc., Wallingford CT, **2009**.

9. Total energies of calculated structures

Table S3. Total electronic energies calculated at different levels of theory, and unscaled zero-point vibrational energies at the B3LYP-D/def2-SVP level (all data in atomic units). Structure symbols with primes (e.g. **D'**, **D''**) refer to less stable conformers of the same compound. For each transition state, the structures connected by it are given in parentheses. Zero-point vibrational energy values are not given for non-optimized structures. Electronic energies with large basis set were not calculated for water adducts. (T) refers to single point triplet calculations, while (SP-S) denotes single point spin-projected energies. The latter were calculated only for copper and B3LYP using $\langle S^2 \rangle$ values in Table S1 for the broken symmetry states, and $\langle S^2 \rangle$=2 for the triplet states. Metal complexes contain copper unless explicitly noted.

	B3LYP-D/ def2-SVP	ZPVE	B3LYP-D/ def2-TZVPP	M06/ def2-TZVPP
1	-1906.9158	0.3895	-1908.3972	-1908.2214
half-**1** (S-S homolytically cleaved)	-953.4183	0.1930	-954.1586	-954.0679
Cu^+	-1639.8932	0.0000	-1640.1350	-1640.1551
2	-952.8734	0.1836	-953.6131	-953.5302
3	-954.0556	0.2064	-954.7979	-954.7138
opened **3** (*E*)	-954.0494	0.2021	-954.7921	-954.7024
A	-3547.0200	0.3921	-3548.7319	-3548.5748
A'	-3547.0200	0.3920	-3548.7317	-3548.5757
TS$_{A/E,Z\text{-}A}$ (**A** / *E,Z*-**A'**)	-3546.9830	0.3901	-3548.6938	-3548.5390
E,Z-**A**	-3547.0112	0.3923	-3548.7257	-3548.5683
E,Z-**A'**	-3547.0080	0.3920	-3548.7216	-3548.5648
TS$_{AB}$ (**A** / **B**)	-3547.0025	0.3907	-3548.7108	-3548.5460
TS$_{AB}$ (**A** / **B**) (T)			-3548.7022	
TS$_{AB}$ (**A** / **B**) (SP-S)			-3548.7131	
B	-3547.0061	0.3912	-3548.7149	-3548.5483
B (T)	-3547.0079		-3548.7166	-3548.5502
B (SP-S)			-3548.7131	
B'	-3547.0029	0.3909	-3548.7127	-3548.5451
TS$_{BC}$ (**B** / **C**)	-3546.9751	0.3898	-3548.6853	-3548.5196
TS$_{BC}$ (**B** / **C**) (T)			-3548.6852	
TS$_{BC}$ (**B** / **C**) (SP-S)			-3548.6853	
C	-3546.9789	0.3900	-3548.6883	-3548.5218
C (T)			-3548.6882	
C (SP-S)			-3548.6883	
TS$_{CD}$ (**C** / **D**)	-3546.9758	0.3895	-3548.6850	-3548.5173
TS$_{CD}$ (**C** / **D**) (T)			-3548.6842	
TS$_{CD}$ (**C** / **D**) (SP-S)			-3548.6857	
D	-3546.9958	0.3908	-3548.7071	-3548.5434
D (T)	-3546.9939		-3548.7052	-3548.5421
D (SP-S)			-3548.7086	
D'	-3546.9953	0.3911	-3548.7056	-3548.5440
D''	-3546.9946	0.3912	-3548.7049	-3548.5437
TS$_{AD}$ (**A'** / **D'**)	-3546.9726	0.3906	-3548.6808	-3548.5221
TSDE$_S$ (**D''** / **E**$_S$)	-3546.9761	0.3865	-3548.6856	-3548.5252
TSDE$_S$ (**D''** / **E**$_S$) (T)			-3548.6710	
TSDE$_S$ (**D''** / **E**$_S$) (SP-S)			-3548.6869	
TSDE$_C$ (**D** / **E**$_C$)	-3546.9638	0.3866	-3548.6728	-3548.5092
TSDE$_C$ (**D** / **E**$_C$) (T)			-3548.6534	

TSDE$_C$ (**D** / **E$_C$**) (SP-S)			-3548.6728	
TSDE$_N$ (**D'** / **E$_N$**)	-3546.9639	0.3870	-3548.6766	-3548.5120
TSDE$_N$ (**D'** / **E$_N$**) (T)			-3548.6593	
TSDE$_N$ (**D'** / **E$_N$**) (SP-S)			-3548.6785	
E$_S$	-3547.0524	0.3902	-3548.7637	-3548.6060
E$_C$	-3547.0257	0.3919	-3548.7352	-3548.5776
E$_N$	-3547.0552	0.3939	-3548.7682	-3548.6110
E$_{Cu}$	-3546.9738	0.3889	-3548.6908	-3548.5264
E$_{NR}$	-3547.0480	0.3933	-3548.7605	-3548.6095
TSBB$_T$ (**B'** / **B$_T$**)	-3546.9681	0.3894	-3548.6786	-3548.5187
TSBB$_T$ (**B'** / **B$_T$**) (T)			-3548.6767	
TSBB$_T$ (**B'** / **B$_T$**) (SP-S)			-3548.6802	
B$_T$	-3546.9757	0.3909	-3548.6867	-3548.5294
B$_T$ (T)	-3546.9581		-3548.6685	-3548.5106
TSB$_T$D$_S$ (**B$_T$** / **D$_S$**)	-3546.9614	0.3884	-3548.6746	-3548.5141
TSB$_T$D$_S$ (**B$_T$** / **D$_S$**) (T)			-3548.6743	
TSB$_T$D$_S$ (**B$_T$** / **D$_S$**) (SP-S)			-3548.6748	
D$_S$	-3546.9630	0.3893	-3548.6780	-3548.5204
D$_S$ (T)	-3546.9629		-3548.6779	-3548.5204
D$_S$ (SP-S)			-3548.6781	
TSD$_S$E$_{SS}$ (**D$_S$** / **E$_{SS}$**)	-3546.9531	0.3870	-3548.6673	-3548.5082
TSD$_S$E$_{SS}$ (**D$_S$** / **E$_{SS}$**) (T)			-3548.6575	
TSD$_S$E$_{SS}$ (**D$_S$** / **E$_{SS}$**) (SP-S)			-3548.6709	
E$_{SS}$	-3547.0258	0.3891	-3548.7397	-3548.5864
TSBE$_{SS}$ (**B'** / **E$_{SS}$**)	-3546.9586	0.3845	-3548.6694	-3548.5083
I	-3546.9417	0.3900	-3548.6558	-3548.4980
I (T)			-3548.6416	
I (SP-S)			-3548.6601	
II	-3546.9575	0.3894	-3548.6659	-3548.5087
II (T)			-3548.6650	
II (SP-S)			-3548.6669	
F$_S$	-2594.0928	0.2034	-2595.0734	-2595.0057
F$_S$'	-2594.0927	0.2034	-2595.0733	-2595.0055
F$_C$	-2594.0688	0.2060	-2595.0474	-2594.9798
F$_N$	-2594.0821	0.2078	-2595.0681	-2594.9983
F$_N$'	-2594.0755	0.2078	-2595.0619	-2594.9919
F$_{Cu}$	-2594.0201	0.2014	-2595.0026	-2594.9258
F$_{Cu}$ (T)			-2594.9980	
F$_{Cu}$ (SP-S)			-2595.0061	
F$_{NR}$	-2594.0791	0.2071	-2595.0590	-2594.9955
F$_S$-H_2O	-2670.4693	0.2288		
F$_C$-H_2O	-2670.4428	0.2312		
F$_N$-H_2O	-2670.4671	0.2323		
F$_{NR}$-H_2O	-2670.4620	0.2327		
TSF$_S$F$_N$ (**F$_S$'** / **F$_N$**)	-2594.0495	0.2027	-2595.0345	-2594.9655
TSF$_N$F$_{NR2}$ (**F$_N$'** / **F$_{NR2}$**)	-2594.0521	0.2062	-2595.0344	-2594.9713
F$_{NR2}$	-2594.0532	0.2067	-2595.0337	-2594.9724

TS$F_{NR2}F_{NR3}$ (**F_{NR2}** / **F_{NR3}**)	-2594.0530	0.2067	-2595.0329	-2594.9715
F_{NR3}	-2594.0541	0.2069	-2595.0348	-2594.9719
TSF_{NR3}G (**F_{NR3}** / **G**)	-2594.0215	0.2015	-2595.0076	-2594.9400
G	-2594.0490	0.2024	-2595.0360	-2594.9726
2-H^+	-953.2528	0.1968	-953.9916	-953.9043
CuH	-1640.7683	0.0042	-1641.0255	-1641.0474
Cu(half-**1**)$^+$	-2593.4759	0.1945	-2594.4542	-2594.3844
$ZnCl^+$	-2238.7639	0.0010	-2239.1820	-2239.2357
ZnCl-**A**	-4145.9203	0.3942	-4147.8051	-4147.6793
ZnCl-**B**	-4145.8814	0.3925	-4147.7588	-4147.6276
ZnCl-**C**	-4145.8756	0.3925	-4147.7534	-4147.6200
ZnCl-**D**	-4145.8998	0.3931	-4147.7780	-4147.6501
ZnCl-**D'**	-4145.8961	0.3928	-4147.7761	-4147.6494
ZnCl-**D''**	-4145.8959	0.3928	-4147.7760	-4147.6487
ZnCl-**TS_{AD}** (ZnCl-**A** / ZnCl-**D'**)	-4145.8766	0.3931	-4147.7575	-4147.6318
ZnCl-**TSDE_S** (ZnCl-**D''** / ZnCl-**E_S**)	-4145.8890	0.3892	-4147.7682	-4147.6398
ZnCl-**E_S**	-4145.9514	0.3923	-4147.8339	-4147.7078
ZnCl-**F_S**	-3193.0007	0.2061	-3194.1547	-3194.1188
Zn(half-**1**)Cl^+	-3192.3846	0.1968	-3193.5359	-3193.4995

10. Cartesian coordinates of calculated structures

B3LYP-D/def2-SVP fully optimized geometries, given in standard XYZ format: coordinates are Cartesian coordinates in the usual order, units are ångstroms, first line indicates total number of atoms, second line is molecule name. Page numbers are omitted in this section to ease copying and pasting.

```
   50
1
 C     2.559323    -1.082275     3.459342
 C     2.035230    -0.859165     2.173926
 C     2.770444    -0.086029     1.251501
 C     3.998850     0.459026     1.618831
 C     4.513171     0.237401     2.905877
 C     3.792910    -0.535162     3.824769
 C     0.726535    -1.417287     1.810094
 N     0.186959    -1.175229     0.679073
 C    -1.103214    -1.576282     0.351113
 C    -1.398940    -1.921023    -0.992098
 C    -2.719783    -2.216941    -1.358599
 C    -3.753247    -2.167442    -0.419018
 C    -3.463593    -1.837149     0.910247
 C    -2.154600    -1.548682     1.290889
 S    -0.081237    -2.128738    -2.189754
 S    -0.106928    -0.366122    -3.363572
 C     1.185933     0.658551    -2.663154
 C     2.469580     0.599995    -3.226940
 C     3.499585     1.421634    -2.759959
 C     3.243946     2.320724    -1.717194
 C     1.975647     2.382572    -1.139368
 C     0.929498     1.548756    -1.588435
 N    -0.338979     1.587974    -1.021447
 C    -0.472376     1.646075     0.247207
 C    -1.785427     1.655600     0.899509
 C    -1.856719     1.678494     2.302639
 C    -3.094902     1.620336     2.948362
 C    -4.270112     1.538948     2.192206
 C    -4.204676     1.519600     0.790555
 C    -2.971694     1.577632     0.145803
 H    -1.939959    -1.233255     2.313458
 H    -4.264287    -1.781518     1.651976
 H    -4.779903    -2.386368    -0.723924
 H    -2.925410    -2.492241    -2.395932
 H     1.769680     3.090682    -0.333534
 H     4.036336     2.981471    -1.353965
 H     4.491882     1.367834    -3.215051
 H     2.649273    -0.104055    -4.042972
 H     0.402611     1.635599     0.924890
 H    -0.930234     1.728573     2.882873
 H    -3.145556     1.636150     4.040529
 H    -5.240217     1.489429     2.695067
 H    -5.123716     1.446643     0.202917
 H    -2.888751     1.535703    -0.942125
 H     0.232976    -2.053200     2.573668
 H     2.360399     0.070344     0.252609
 H     4.558654     1.058830     0.896028
 H     5.478331     0.665304     3.191275
 H     4.193908    -0.711275     4.826550
 H     1.990150    -1.686736     4.172518
```

```
  25
half-1
 C    -2.955515     1.549453     0.153928
 C    -1.780103     1.525633     0.931567
 C    -1.876168     1.577649     2.333467
 C    -3.125775     1.662296     2.953452
 C    -4.288372     1.689416     2.174579
 C    -4.200294     1.630863     0.774817
 C    -0.458530     1.442140     0.300522
 N    -0.296222     1.443370    -0.966158
 C     0.953259     1.460672    -1.554301
 C     1.225743     0.575304    -2.659905
 C     2.511446     0.642921    -3.269706
 C     3.474835     1.546541    -2.842121
 C     3.190948     2.409808    -1.766885
 C     1.949891     2.363000    -1.130906
 S     0.052229    -0.545256    -3.227087
 H     1.722742     3.048431    -0.310909
 H     3.946145     3.122731    -1.424063
 H     4.449006     1.586346    -3.336133
 H     2.714633    -0.043841    -4.094774
 H     0.405939     1.362618     0.991764
 H    -0.961939     1.552998     2.934562
 H    -3.194751     1.704709     4.043686
 H    -5.267436     1.752703     2.657767
 H    -5.111193     1.645787     0.170247
 H    -2.856832     1.492494    -0.932566
  24
2
 C    -0.008488    -0.655266    -2.004452
 C     0.000201     0.739869    -1.725889
 C     0.005545     1.657258    -2.793406
 C     0.002351     1.176281    -4.099850
 C    -0.006192    -0.209565    -4.361115
 C    -0.011734    -1.138456    -3.319347
 N     0.002568     1.069421    -0.390734
 C    -0.004070     0.021460     0.374451
 H     0.011962     2.726849    -2.572485
 H     0.006444     1.880089    -4.936272
 H    -0.008502    -0.563889    -5.395271
 H    -0.018359    -2.211202    -3.526496
 S    -0.013908    -1.539267    -0.498410
 C    -0.003351     0.076445     1.845204
 C    -0.016745    -1.084745     2.640486
 C    -0.015743    -0.989885     4.033934
 C    -0.001295     0.264983     4.653216
 C     0.012093     1.426399     3.869134
 C     0.011137     1.336237     2.477551
 H    -0.028374    -2.072131     2.170842
 H    -0.026385    -1.900721     4.638295
 H    -0.000580     0.338553     5.744136
 H     0.023466     2.409442     4.347947
 H     0.021627     2.230278     1.851367
  26
3
 C     0.146039     0.633361     1.955081
 C    -0.278642    -0.699263     1.753671
 C    -0.391572    -1.565750     2.843797
 C    -0.061952    -1.097740     4.126343
```

```
 C     0.370777     0.216785     4.320161
 C     0.476492     1.093992     3.225909
 N    -0.502847    -1.009372     0.416301
 C    -0.743194     0.150210    -0.429741
 H    -0.727344    -2.595870     2.694563
 H    -0.151946    -1.773661     4.980932
 H     0.621556     0.571058     5.323071
 H     0.806453     2.125958     3.370843
 S     0.234375     1.511996     0.410544
 C    -0.311612    -0.047133    -1.862363
 C    -1.091455     0.470101    -2.905351
 C    -0.687454     0.316452    -4.236735
 C     0.499805    -0.361509    -4.531373
 C     1.281801    -0.883212    -3.491205
 C     0.880614    -0.723978    -2.163254
 H    -2.022348     0.995228    -2.669437
 H    -1.302994     0.723099    -5.043792
 H     0.816615    -0.486009    -5.570617
 H     2.210122    -1.414346    -3.719330
 H     1.478565    -1.121580    -1.340202
 H    -1.807530     0.462672    -0.413278
 H    -1.068528    -1.825570     0.207511
   26
opened 3 (E)
 C    -0.804891    -0.564405    -2.627923
 C     0.381501     0.081705    -2.225194
 C     1.234690     0.622704    -3.204459
 C     0.909416     0.528543    -4.560294
 C    -0.272967    -0.110730    -4.950034
 C    -1.128192    -0.657203    -3.980359
 C     0.749282     0.202429    -0.809879
 N    -0.005368    -0.192157     0.145168
 C     0.401264    -0.133236     1.480507
 C    -0.583080     0.079772     2.485143
 C    -0.193722     0.113597     3.834239
 C     1.140648    -0.073225     4.200922
 C     2.112682    -0.305077     3.219701
 C     1.739910    -0.335136     1.876480
 S    -2.293203     0.339709     2.088765
 H    -0.951145     0.283192     4.604574
 H     1.417636    -0.052128     5.258271
 H     3.154797    -0.476636     3.501246
 H     2.485217    -0.550412     1.106545
 H    -2.130088     0.101278     0.764091
 H     1.733274     0.672979    -0.611719
 H     2.157135     1.122081    -2.892192
 H     1.577534     0.953655    -5.313987
 H    -0.529566    -0.187030    -6.010307
 H    -2.049224    -1.160217    -4.287526
 H    -1.452434    -0.989825    -1.858205
   51
A
   C  -2.708742   2.786570   1.410251
   C  -3.602655   1.734453   1.708612
   C  -4.319611   1.765972   2.923513
   C  -4.177166   2.839930   3.800927
   C  -3.295225   3.881711   3.486996
   C  -2.555075   3.847589   2.297006
   C  -3.756262   0.567120   0.856920
```

```
   N  -3.418911   0.491507  -0.395923
   C  -3.364514  -0.785890  -1.014833
   C  -3.535891  -0.925323  -2.420220
   C  -3.459699  -2.195325  -3.015449
   C  -3.214699  -3.334455  -2.246636
   C  -3.003245  -3.199432  -0.871213
   C  -3.061997  -1.941643  -0.268810
   S  -3.884173   0.450193  -3.495095
   S  -1.839300   1.357880  -3.541138
  Cu  -3.350755   2.094523  -1.590196
   N  -3.351403   3.888252  -2.474472
   C  -3.494046   4.996003  -1.809855
   C  -4.180912   5.140816  -0.537528
   C  -3.952545   6.317484   0.207025
   C  -4.616326   6.530289   1.414327
   C  -5.537414   5.582309   1.877604
   C  -5.795520   4.423566   1.132098
   C  -5.120733   4.198900  -0.063712
   C  -2.909617   3.951210  -3.823122
   C  -3.195003   5.070885  -4.628520
   C  -2.766247   5.138749  -5.955152
   C  -2.065221   4.072382  -6.526228
   C  -1.821001   2.928695  -5.763939
   C  -2.233972   2.852563  -4.423496
   H  -3.792870   5.889199  -4.223115
   H  -3.003751   6.023864  -6.550468
   H  -1.735623   4.117077  -7.566680
   H  -1.305282   2.072333  -6.204104
   H  -3.088955   5.929715  -2.230825
   H  -5.346841   3.312213  -0.661204
   H  -6.529468   3.697590   1.487855
   H  -6.068562   5.752935   2.817387
   H  -4.427243   7.439505   1.989960
   H  -3.246965   7.063212  -0.170822
   H  -3.592528  -2.277637  -4.096490
   H  -3.160895  -4.315500  -2.723948
   H  -2.767709  -4.075169  -0.261428
   H  -2.833814  -1.853186   0.794926
   H  -4.178027  -0.321154   1.353140
   H  -4.991623   0.939221   3.171724
   H  -4.742393   2.861558   4.735714
   H  -3.172106   4.718401   4.179246
   H  -1.854466   4.652748   2.066492
   H  -2.106554   2.743266   0.499330
   51
A'
   C  -2.826422   2.849465  -4.599978
   C  -3.355070   3.913404  -3.821835
   C  -4.046706   4.947616  -4.474460
   C  -4.182263   4.953928  -5.864436
   C  -3.634993   3.921160  -6.632213
   C  -2.965665   2.872950  -5.996921
   N  -3.221231   3.889472  -2.404637
   C  -3.076015   5.002085  -1.757768
   C  -2.973760   5.139242  -0.309839
   C  -3.373174   6.369974   0.253263
   C  -3.367601   6.550501   1.636379
   C  -2.926237   5.516817   2.472031
   C  -2.479820   4.308340   1.921406
```

```
   C  -2.503611   4.117846   0.542422
   S  -1.941495   1.480549  -3.870456
  Cu  -3.351367   2.094270  -1.602457
   S  -3.672984   0.143460  -3.492040
   C  -2.911569  -0.931684  -2.286176
   C  -2.949441  -0.657352  -0.893346
   C  -2.318959  -1.551240  -0.011831
   C  -1.696733  -2.707528  -0.487378
   C  -1.685424  -2.991563  -1.856695
   C  -2.287197  -2.101152  -2.748612
   N  -3.577369   0.530592  -0.423560
   C  -4.192063   0.522911   0.716324
   C  -4.845988   1.669318   1.336173
   C  -5.363064   2.760885   0.607161
   C  -5.934912   3.842459   1.271880
   C  -5.997222   3.854230   2.671433
   C  -5.515168   2.763848   3.406615
   C  -4.960653   1.669804   2.742471
   H  -4.509540   5.741589  -3.885026
   H  -4.730784   5.766910  -6.346621
   H  -3.739952   3.923340  -7.719460
   H  -2.541285   2.053211  -6.580947
   H  -3.046786   5.946918  -2.322866
   H  -2.122866   3.184920   0.119137
   H  -2.109850   3.514244   2.573446
   H  -2.910514   5.660324   3.555433
   H  -3.696485   7.500654   2.064008
   H  -3.707540   7.178795  -0.402920
   H  -2.278726  -2.303018  -3.822088
   H  -1.199108  -3.895037  -2.231410
   H  -1.207618  -3.383148   0.218654
   H  -2.290098  -1.324573   1.055895
   H  -4.221544  -0.410533   1.299713
   H  -4.592428   0.812170   3.313015
   H  -5.582582   2.763390   4.497125
   H  -6.442231   4.707606   3.189437
   H  -6.338382   4.680918   0.699755
   H  -5.348695   2.743170  -0.485265
   51
TS A/E,Z-A
 C     1.746492     2.724379     1.453723
 C     2.892590     1.983211     1.811323
 C     3.598968     2.328372     2.980891
 C     3.196184     3.419139     3.752081
 C     2.064156     4.156245     3.382041
 C     1.335265     3.801720     2.237246
 C     3.336633     0.826374     1.042757
 N     3.119330     0.657889    -0.223819
 C     3.416470    -0.592699    -0.830974
 C     3.852403    -0.655109    -2.184262
 C     4.105234    -1.906662    -2.770841
 C     3.939399    -3.087876    -2.043613
 C     3.491586    -3.027169    -0.720422
 C     3.223358    -1.792068    -0.125247
 S     4.186846     0.791470    -3.165649
 S     2.030347     1.413336    -3.704341
Cu     2.729245     2.151980    -1.473951
 N     2.837615     3.915248    -2.255919
 C     3.096282     4.403268    -1.074078
```

```
 C     4.433888     4.531739    -0.506268
 C     4.568862     5.011232     0.811903
 C     5.836808     5.157614     1.374313
 C     6.972888     4.821821     0.626605
 C     6.844165     4.334226    -0.685446
 C     5.582147     4.184301    -1.251648
 C     2.600586     4.116614    -3.575114
 C     2.715387     5.398567    -4.164251
 C     2.510845     5.551613    -5.530466
 C     2.203097     4.453860    -6.358074
 C     2.097657     3.187254    -5.798183
 C     2.272141     3.003037    -4.409823
 H     2.969289     6.252646    -3.533251
 H     2.596699     6.550186    -5.967682
 H     2.050443     4.596398    -7.429649
 H     1.863476     2.320054    -6.420472
 H     2.268299     4.763972    -0.434194
 H     5.460727     3.793921    -2.264759
 H     7.736291     4.073296    -1.259900
 H     7.967025     4.937876     1.066335
 H     5.942852     5.532282     2.395206
 H     3.673611     5.255815     1.388413
 H     4.438819    -1.941341    -3.810362
 H     4.140192    -4.051788    -2.516730
 H     3.327814    -3.945449    -0.151283
 H     2.822638    -1.757557     0.890037
 H     3.892238     0.054650     1.598533
 H     4.473186     1.740850     3.275372
 H     3.755477     3.687361     4.651609
 H     1.735419     4.997468     3.997923
 H     0.431587     4.356083     1.971206
 H     1.150550     2.417988     0.589595
   51
E,Z-A
   C  -2.472264   4.373133  -1.718337
   C  -1.774085   3.324368  -1.081369
   C  -0.398494   3.489628  -0.810069
   C   0.253711   4.665523  -1.167900
   C  -0.452828   5.698809  -1.803677
   C  -1.816944   5.551273  -2.077901
   C  -2.538603   2.132603  -0.743253
   N  -2.084742   1.048621  -0.198443
   C  -2.992099   0.010198   0.148564
   C  -2.610596  -1.346305  -0.018391
   C  -3.496139  -2.371213   0.347319
   C  -4.741625  -2.069616   0.901512
   C  -5.116189  -0.732396   1.077325
   C  -4.250779   0.297206   0.704143
   S  -1.052586  -1.774664  -0.784396
  Cu  -0.229572   0.506519   0.177238
   S   0.059078  -2.611804   0.922508
   C   1.699227  -2.196196   0.355550
   C   2.249182  -0.900768   0.505051
   C   3.549777  -0.642441   0.051574
   C   4.318397  -1.663102  -0.511059
   C   3.792510  -2.954087  -0.637286
   C   2.486635  -3.212292  -0.215114
   N   1.481274   0.169544   1.044818
   C   1.817064   0.782798   2.137635
```

```
   C   2.852207   0.488905   3.126408
   C   3.172359   1.536817   4.019141
   C   4.132108   1.359344   5.014876
   C   4.764345   0.118309   5.153589
   C   4.432524  -0.941210   4.296000
   C   3.490866  -0.763296   3.285183
   H   3.954966   0.366145   0.157962
   H   5.333192  -1.446422  -0.854144
   H   4.391576  -3.754770  -1.076901
   H   2.055610  -4.210190  -0.323491
   H   1.214490   1.671639   2.368877
   H   3.240085  -1.600350   2.636021
   H   4.912904  -1.914637   4.420461
   H   5.509966  -0.030180   5.938983
   H   4.379086   2.182079   5.689952
   H   2.661342   2.499227   3.921524
   H  -3.199841  -3.410768   0.188327
   H  -5.418556  -2.876047   1.192588
   H  -6.085806  -0.486902   1.517461
   H  -4.534054   1.337690   0.876663
   H  -3.609815   2.180061  -0.994835
   H  -3.538951   4.254765  -1.930429
   H  -2.368619   6.354384  -2.572077
   H   0.064616   6.619702  -2.084964
   H   1.319047   4.784527  -0.955394
   H   0.163894   2.692111  -0.313933
  51
E,Z-A'
   C   1.132724  -2.601023   0.857163
   C   1.942356  -1.437222   0.939875
   C   3.308972  -1.587393   1.240427
   C   3.866688  -2.851835   1.412378
   C   3.075161  -4.002535   1.283749
   C   1.715507  -3.874435   1.006081
   N   1.354870  -0.160432   0.838994
   C   1.902968   0.869345   0.257692
   C   3.024836   0.957751  -0.674507
   C   3.643850   2.218168  -0.815764
   C   4.697358   2.395611  -1.713462
   C   5.118697   1.323754  -2.508837
   C   4.483165   0.076031  -2.406656
   C   3.448817  -0.112358  -1.494019
   S  -0.639961  -2.535789   0.748178
  Cu  -0.610256  -0.043334   0.711807
   S  -1.047783  -1.813624  -1.325946
   C  -2.780881  -1.441272  -1.096680
   C  -3.243624  -0.247767  -0.477311
   C  -4.626883  -0.032321  -0.369850
   C  -5.539950  -0.953388  -0.890482
   C  -5.085107  -2.116176  -1.518282
   C  -3.711589  -2.358557  -1.610131
   N  -2.323441   0.693842   0.059408
   C  -2.562568   1.958785  -0.084333
   C  -1.753059   3.038436   0.470237
   C  -0.872282   2.867052   1.560694
   C  -0.096019   3.932632   2.011662
   C  -0.191006   5.186387   1.387201
   C  -1.079866   5.375872   0.322563
   C  -1.865030   4.311703  -0.125273
```

```
   H   3.928515  -0.695270   1.341862
   H   4.929427  -2.941430   1.650883
   H   3.515182  -4.994271   1.410319
   H   1.082188  -4.760093   0.917293
   H   1.417418   1.831786   0.476250
   H   2.955921  -1.082494  -1.425937
   H   4.798833  -0.751022  -3.047224
   H   5.936177   1.461089  -3.221366
   H   5.182181   3.370699  -1.802846
   H   3.293606   3.057588  -0.207892
   H  -3.342865  -3.269517  -2.086858
   H  -5.794655  -2.842143  -1.921742
   H  -6.611468  -0.764584  -0.789069
   H  -4.988081   0.854501   0.155670
   H  -3.418985   2.271611  -0.702669
   H  -2.563731   4.457843  -0.954128
   H  -1.165499   6.355471  -0.153880
   H   0.416234   6.021301   1.746468
   H   0.570828   3.796025   2.866636
   H  -0.823488   1.905487   2.080192
   51
TS AB
 C     4.694788    -0.377464    -1.026185
 C     3.303374    -0.574708    -0.905922
 C     2.795518    -1.210537     0.248087
 C     3.665318    -1.672952     1.231901
 C     5.050417    -1.498910     1.086208
 C     5.563473    -0.846553    -0.041483
 C     2.442185    -0.056267    -1.956355
 N     1.227652    -0.452591    -2.174192
 C     0.382737     0.227481    -3.081857
 C    -0.813573    -0.432026    -3.512723
 C    -1.736283     0.260113    -4.330018
 C    -1.469067     1.554771    -4.764813
 C    -0.297098     2.200082    -4.343643
 C     0.606109     1.549770    -3.499084
 S    -1.150772    -2.102796    -3.125322
Cu     0.426425    -2.275911    -1.539745
 S    -1.187429    -2.626347    -0.021830
 C    -0.678389    -4.247614     0.388760
 C     0.602342    -4.766783     0.012073
 C     0.957375    -6.054542     0.445966
 C     0.099553    -6.803044     1.255775
 C    -1.155129    -6.295188     1.623878
 C    -1.549779    -5.039881     1.170692
 N     1.401709    -3.995399    -0.863495
 C     2.661386    -4.251551    -1.028106
 C     3.504419    -3.637663    -2.041013
 C     2.980924    -3.061169    -3.218890
 C     3.836912    -2.502278    -4.164060
 C     5.224787    -2.519641    -3.955469
 C     5.756413    -3.111960    -2.803564
 C     4.902314    -3.677335    -1.857492
 H     1.894071    -6.506968     0.115679
 H     0.399359    -7.805224     1.571569
 H    -1.832806    -6.891764     2.238887
 H    -2.535932    -4.643692     1.423529
 H     1.470398     2.104173    -3.128990
 H    -0.100622     3.231696    -4.645670
```

```
 H    -2.184158     2.073803    -5.407130
 H    -2.659442    -0.244542    -4.624520
 H     2.889505     0.726763    -2.588491
 H     5.089559     0.132269    -1.908980
 H     6.640765    -0.699140    -0.147755
 H     5.729069    -1.853907     1.866395
 H     3.265345    -2.150177     2.130124
 H     1.717023    -1.308549     0.387354
 H     3.166494    -4.979985    -0.374795
 H     1.905673    -3.084862    -3.407450
 H     3.426844    -2.071742    -5.081118
 H     5.893757    -2.089365    -4.705524
 H     6.837532    -3.137476    -2.648274
 H     5.311549    -4.140764    -0.955945
   51
B
 C     4.709749    -3.113511    -2.474257
 C     3.338810    -3.424765    -2.358533
 C     2.557132    -3.537787    -3.527331
 C     3.130809    -3.313115    -4.775808
 C     4.490714    -2.978487    -4.877684
 C     5.280776    -2.883703    -3.725677
 C     2.807725    -3.631711    -1.022115
 N     1.553945    -3.654029    -0.693819
 C     1.198385    -4.001993     0.621702
 C     0.025990    -3.410616     1.202781
 C    -0.327728    -3.741873     2.536230
 C     0.426475    -4.649297     3.268062
 C     1.551730    -5.255156     2.680315
 C     1.927759    -4.938428     1.372941
 S    -0.971656    -2.304397     0.316335
Cu    -0.043895    -2.670494    -1.725292
 S    -1.333405    -3.628736    -3.332775
 C    -1.407398    -2.253570    -4.386562
 C    -0.552475    -1.114842    -4.202256
 C    -0.703447    -0.008922    -5.054825
 C    -1.635855    -0.029994    -6.094326
 C    -2.450977    -1.157204    -6.301621
 C    -2.339254    -2.252766    -5.456129
 N     0.377966    -1.126854    -3.148084
 C     1.504755    -0.503384    -3.293462
 C     2.508599    -0.301396    -2.262579
 C     3.795582     0.102984    -2.674181
 C     4.810696     0.295312    -1.737502
 C     4.545818     0.102662    -0.376325
 C     3.260992    -0.273703     0.046424
 C     2.247438    -0.472197    -0.887141
 H     2.780000    -5.446904     0.917873
 H     2.133290    -5.989517     3.243221
 H     0.136474    -4.903671     4.290036
 H    -1.214249    -3.275149     2.971512
 H    -0.106964     0.889244    -4.882093
 H    -1.737716     0.844515    -6.741917
 H    -3.181237    -1.164947    -7.114022
 H    -2.976587    -3.129481    -5.593400
 H     1.767101    -0.095763    -4.283715
 H     3.996269     0.248785    -3.738959
 H     5.807123     0.600621    -2.065488
 H     5.336723     0.263229     0.361295
```

```
 H     3.050186    -0.396523     1.111880
 H     1.245012    -0.744907    -0.557172
 H     3.569316    -3.755149    -0.234571
 H     1.506486    -3.817422    -3.450415
 H     2.523322    -3.413124    -5.678802
 H     4.937612    -2.809285    -5.861028
 H     6.341748    -2.635687    -3.805992
 H     5.319666    -3.037256    -1.570232
   51
B'
 C    -1.766152    -1.258571    -1.564627
 C    -1.572792    -2.135298    -0.476468
 C    -1.401065    -3.515444    -0.722726
 C    -1.380658    -3.999635    -2.030355
 C    -1.554236    -3.114767    -3.103412
 C    -1.755036    -1.746289    -2.867928
 C    -1.560407    -1.681638     0.902440
 N    -1.342397    -0.463041     1.294418
 C    -1.479835    -0.136411     2.656686
 C    -0.655612     0.905166     3.204129
 C    -0.769917     1.222085     4.582759
 C    -1.689023     0.566334     5.391230
 C    -2.521114    -0.423647     4.839046
 C    -2.419365    -0.766175     3.487929
 S     0.467803     1.787936     2.226116
Cu    -0.288841     1.023681     0.203802
 S    -1.136996     2.460487    -1.331307
 C    -0.429506     1.724509    -2.739896
 C     0.572079     0.707615    -2.628664
 C     1.047844     0.085355    -3.794071
 C     0.583671     0.478010    -5.050269
 C    -0.372619     1.502665    -5.168564
 C    -0.864735     2.124884    -4.027196
 N     1.023807     0.342764    -1.349630
 C     2.271467     0.034043    -1.184955
 C     2.870900    -0.478540     0.036417
 C     2.112962    -1.033571     1.089130
 C     2.746082    -1.493820     2.240458
 C     4.142087    -1.407699     2.359202
 C     4.906773    -0.876938     1.313420
 C     4.275481    -0.424536     0.153736
 H    -3.099305    -1.510143     3.067512
 H    -3.264101    -0.924747     5.464513
 H    -1.776101     0.830698     6.447536
 H    -0.127984     2.005779     4.991291
 H     1.767535    -0.731229    -3.707923
 H     0.965520    -0.018910    -5.945498
 H    -0.730674     1.808636    -6.154157
 H    -1.607231     2.922628    -4.104667
 H     2.972534     0.189329    -2.022300
 H     4.868267    -0.012610    -0.668239
 H     5.994151    -0.819019     1.402280
 H     4.634556    -1.766637     3.266736
 H     2.155807    -1.927726     3.051651
 H     1.034310    -1.118152     0.982900
 H    -1.718693    -2.467267     1.660180
 H    -1.949867    -0.201416    -1.376091
 H    -1.905540    -1.059883    -3.704285
 H    -1.546477    -3.495389    -4.128190
```

```
 H    -1.237539    -5.066689    -2.216563
 H    -1.274429    -4.202068     0.119562
   51
TS BC
 C    -0.925616    -5.425616     2.967462
 C    -0.377691    -5.356169     1.654232
 C     0.537942    -4.286655     1.378487
 C     0.856834    -3.348741     2.360714
 C     0.295335    -3.449876     3.640707
 C    -0.599265    -4.489479     3.941992
 N     1.084196    -4.136251     0.071801
 C     2.092942    -4.858588    -0.275150
 S    -0.834247    -6.503763     0.453087
Cu     0.049596    -2.870477    -1.017573
 S    -1.974631    -2.616860    -1.992464
 C    -1.611439    -1.225569    -2.948649
 C    -0.303705    -0.621128    -2.950204
 C    -0.101817     0.555876    -3.690295
 C    -1.135235     1.105863    -4.451524
 C    -2.405769     0.497668    -4.486395
 C    -2.638000    -0.653144    -3.748994
 N     0.707447    -1.198488    -2.175591
 C     1.950998    -1.102569    -2.530234
 C     3.075213    -1.470675    -1.685333
 C     4.334270    -1.671293    -2.285638
 C     5.437744    -2.018830    -1.506925
 C     5.299094    -2.146854    -0.119795
 C     4.054064    -1.926106     0.490011
 C     2.948901    -1.590584    -0.285661
 H     2.563612    -5.511269     0.477314
 H     0.866747     1.058267    -3.649296
 H    -0.953585     2.020640    -5.021409
 H    -3.207256     0.935840    -5.085327
 H    -3.618537    -1.134732    -3.760310
 H     2.203984    -0.725727    -3.535885
 H     4.435917    -1.568107    -3.369281
 H     6.408799    -2.185180    -1.978790
 H     6.166644    -2.405342     0.493051
 H     3.957480    -2.006754     1.575851
 H     1.980156    -1.398569     0.179380
 H     1.553424    -2.542658     2.121745
 H     0.561046    -2.715781     4.405584
 H    -1.035830    -4.564673     4.940639
 H    -1.617277    -6.242274     3.186061
 C     2.695912    -4.850019    -1.604003
 C     4.054086    -5.200638    -1.720968
 C     4.686064    -5.167572    -2.964556
 C     3.959416    -4.813092    -4.107399
 C     2.595787    -4.501272    -4.007083
 C     1.965692    -4.521484    -2.764460
 H     4.616428    -5.481342    -0.826423
 H     5.743940    -5.428438    -3.046182
 H     4.449891    -4.804498    -5.084477
 H     2.020421    -4.266699    -4.906158
 H     0.889337    -4.340608    -2.698410
   51
C
 C    -2.660005    -0.812545     4.535048
 C    -1.571448    -1.122504     3.666519
```

```
 C    -1.442459    -0.342723     2.457184
 C    -2.397979     0.642266     2.162023
 C    -3.451350     0.911062     3.035757
 C    -3.582574     0.177490     4.229095
 N    -0.420392    -0.568364     1.517437
 C     0.795621    -0.789812     1.924128
 S    -0.551253    -2.455850     4.050167
Cu    -0.934531    -0.451297    -0.400254
 S    -2.135013    -1.450700    -2.032131
 C    -1.739684    -0.365695    -3.317481
 C    -0.808911     0.717199    -3.137341
 C    -0.587378     1.607227    -4.202087
 C    -1.222117     1.419517    -5.430899
 C    -2.103824     0.337844    -5.626763
 C    -2.352907    -0.544756    -4.587149
 N    -0.185736     0.877024    -1.895540
 C     1.017303     1.356133    -1.822504
 C     1.665371     1.787562    -0.595061
 C     3.066167     1.947966    -0.594249
 C     3.724874     2.381904     0.555855
 C     2.988985     2.680808     1.709002
 C     1.591764     2.546668     1.711429
 C     0.932927     2.103307     0.568474
 H     1.054914    -0.597327     2.972816
 H     0.070923     2.466056    -4.055937
 H    -1.032403     2.122581    -6.245966
 H    -2.594525     0.198817    -6.592710
 H    -3.035902    -1.386722    -4.722040
 H     1.616062     1.454841    -2.744072
 H     3.634020     1.718592    -1.500092
 H     4.811385     2.495097     0.553615
 H     3.502637     3.035365     2.606651
 H     1.018844     2.802070     2.606504
 H    -0.153340     2.009995     0.558555
 H    -2.299284     1.212229     1.233544
 H    -4.171661     1.695407     2.790532
 H    -4.408017     0.385601     4.913801
 H    -2.754332    -1.393232     5.455074
 C     1.897286    -1.168668     1.051725
 C     3.208252    -0.883830     1.480797
 C     4.299601    -1.176247     0.662664
 C     4.095121    -1.775270    -0.586029
 C     2.796504    -2.095954    -1.009586
 C     1.705542    -1.802227    -0.194784
 H     3.362030    -0.412042     2.454471
 H     5.312284    -0.942588     0.999569
 H     4.950411    -2.016657    -1.222711
 H     2.641845    -2.600701    -1.966584
 H     0.703649    -2.118728    -0.500955
   51
TS CD
 C     1.045552    -5.672761     3.303149
 C     1.305779    -5.428078     1.925886
 C     0.813143    -4.196986     1.341689
 C     0.072374    -3.293440     2.135279
 C    -0.163555    -3.568932     3.472138
 C     0.322398    -4.765227     4.056697
 N     1.011126    -3.973304     0.004307
 C     2.084860    -4.531239    -0.565489
```

```
 S     2.099804    -6.577891     0.931763
Cu    -0.056489    -2.693573    -1.054949
 S    -1.900160    -2.260791    -2.254322
 C    -1.231473    -1.042737    -3.288892
 C     0.102604    -0.531791    -3.113035
 C     0.534906     0.534340    -3.922322
 C    -0.291543     1.053041    -4.918258
 C    -1.581692     0.525864    -5.126167
 C    -2.041661    -0.509186    -4.326531
 N     0.900411    -1.080394    -2.108012
 C     2.194365    -1.065231    -2.176093
 C     3.058972    -1.424924    -1.062050
 C     4.392231    -1.798460    -1.325187
 C     5.227529    -2.205324    -0.284077
 C     4.745887    -2.219412     1.032612
 C     3.432169    -1.811094     1.309484
 C     2.595612    -1.413471     0.270251
 H     3.036628    -4.496390    -0.017115
 H     1.520359     0.973587    -3.753887
 H     0.067058     1.877714    -5.539430
 H    -2.221773     0.937544    -5.909907
 H    -3.042625    -0.922205    -4.472150
 H     2.694700    -0.791648    -3.120650
 H     4.759004    -1.789613    -2.355169
 H     6.257291    -2.505318    -0.493443
 H     5.402514    -2.532066     1.848717
 H     3.065104    -1.801953     2.338309
 H     1.574162    -1.086720     0.475863
 H    -0.301435    -2.373294     1.678527
 H    -0.725115    -2.857529     4.082643
 H     0.125176    -4.970770     5.111526
 H     1.420071    -6.595316     3.751520
 C     2.175708    -4.738386    -2.004394
 C     3.446680    -4.756598    -2.612168
 C     3.563999    -4.903326    -3.994460
 C     2.413113    -5.044473    -4.782580
 C     1.144707    -5.053882    -4.184707
 C     1.024502    -4.912024    -2.803214
 H     4.337072    -4.639981    -1.989808
 H     4.551745    -4.913253    -4.462106
 H     2.506091    -5.164809    -5.865093
 H     0.250731    -5.191597    -4.797699
 H     0.040871    -4.967020    -2.329739
   51
D
 C     0.971632    -5.871592     3.137678
 C     1.358736    -5.324626     1.907926
 C     0.684093    -4.164716     1.377561
 C    -0.389275    -3.580448     2.110535
 C    -0.753455    -4.132777     3.321961
 C    -0.076302    -5.272063     3.836000
 N     1.115150    -3.723970     0.190369
 C     2.276705    -4.426481    -0.310165
 S     2.583820    -5.899178     0.822155
Cu     0.270763    -2.464733    -1.017976
 S    -1.599059    -2.231911    -2.255408
 C    -1.023509    -0.977460    -3.308339
 C     0.277700    -0.392688    -3.150097
 C     0.646598     0.695604    -3.959866
```

```
 C    -0.218602     1.169890    -4.945154
 C    -1.477574     0.569344    -5.138947
 C    -1.870558    -0.494022    -4.338169
 N     1.119273    -0.910495    -2.160103
 C     2.408894    -0.859979    -2.261289
 C     3.308412    -1.209216    -1.168066
 C     4.617088    -1.634166    -1.470213
 C     5.478191    -2.040286    -0.449130
 C     5.049496    -1.994961     0.884676
 C     3.763293    -1.529133     1.197986
 C     2.896944    -1.137507     0.179611
 H     3.164229    -3.785059    -0.164246
 H     1.610537     1.184192    -3.801708
 H     0.085715     2.013812    -5.569255
 H    -2.148696     0.944534    -5.915094
 H    -2.846928    -0.964051    -4.477400
 H     2.875075    -0.565603    -3.216535
 H     4.944590    -1.666988    -2.512924
 H     6.486889    -2.385451    -0.688865
 H     5.726314    -2.305797     1.684663
 H     3.442990    -1.467237     2.240788
 H     1.898489    -0.763260     0.414988
 H    -0.900449    -2.708282     1.695766
 H    -1.571724    -3.692871     3.896811
 H    -0.386383    -5.688639     4.797399
 H     1.477481    -6.751584     3.540235
 C     2.163832    -4.793336    -1.771237
 C     3.281314    -4.670105    -2.607971
 C     3.179566    -4.983489    -3.967737
 C     1.957684    -5.414101    -4.497358
 C     0.839359    -5.541464    -3.663427
 C     0.942591    -5.239492    -2.303248
 H     4.229296    -4.321096    -2.190751
 H     4.054545    -4.888154    -4.615825
 H     1.876787    -5.654475    -5.560477
 H    -0.114779    -5.882502    -4.072880
 H     0.072757    -5.342346    -1.650027
   51
D'
 C    -4.537938    -1.335737     2.244689
 C    -3.195059    -1.298756     1.851106
 C    -2.552011    -0.043652     1.544621
 C    -3.301288     1.165341     1.639431
 C    -4.623727     1.108531     2.030532
 C    -5.242129    -0.134889     2.334153
 N    -1.267527    -0.111156     1.170513
 C    -0.713740    -1.448727     1.216119
 S    -2.115393    -2.637660     1.620477
Cu    -0.295805     1.297784     0.226325
 S    -0.536368     3.115422    -1.079543
 C     0.547002     2.515585    -2.302893
 C     1.500778     1.479120    -2.020093
 C     2.263757     0.949558    -3.072246
 C     2.150186     1.469076    -4.362475
 C     1.262480     2.527387    -4.633560
 C     0.474900     3.047437    -3.615118
 N     1.599693     1.020739    -0.695110
 C     2.716164     0.563752    -0.237200
 C     2.926303     0.016114     1.095858
```

C	4.094468	-0.744864	1.308054
C	4.329455	-1.359230	2.538723
C	3.411672	-1.197889	3.584004
C	2.265254	-0.410187	3.396743
C	2.024051	0.191918	2.163847
H	-0.020871	-1.521125	2.074450
H	2.935211	0.112087	-2.879071
H	2.759322	1.049599	-5.167123
H	1.185982	2.933230	-5.644876
H	-0.227288	3.860460	-3.813015
H	3.608600	0.568852	-0.884068
H	4.809798	-0.868059	0.489756
H	5.231363	-1.957672	2.687741
H	3.596981	-1.669977	4.552210
H	1.565506	-0.258187	4.222619
H	1.137404	0.815731	2.038387
H	-2.808308	2.109805	1.398881
H	-5.206621	2.028962	2.111224
H	-6.290416	-0.150532	2.641716
H	-5.024937	-2.285875	2.473935
C	0.031822	-1.825680	-0.042876
C	1.262942	-2.483299	0.045581
C	1.973716	-2.801202	-1.117494
C	1.455060	-2.458208	-2.370584
C	0.219457	-1.802552	-2.462031
C	-0.492204	-1.492353	-1.302796
H	1.679140	-2.726332	1.026700
H	2.934408	-3.317417	-1.042683
H	2.008902	-2.709004	-3.279223
H	-0.188382	-1.535559	-3.439874
H	-1.456166	-0.980523	-1.367554

51

D''

C	-0.746958	-3.937535	2.836948
C	-0.577317	-3.348295	1.580249
C	0.428517	-2.338546	1.375628
C	1.253531	-1.938414	2.464357
C	1.077350	-2.536279	3.697154
C	0.081893	-3.529408	3.885720
N	0.490533	-1.809944	0.147399
C	-0.418531	-2.429789	-0.806671
S	-1.483618	-3.650634	0.124138
Cu	1.300408	-0.133386	-0.435560
S	2.855372	0.625020	-1.910525
C	1.882927	1.944411	-2.475005
C	0.759623	2.418447	-1.717101
C	-0.035888	3.452431	-2.237106
C	0.282892	4.041508	-3.459829
C	1.404761	3.606657	-4.193674
C	2.199890	2.581220	-3.702569
N	0.476134	1.812876	-0.486529
C	0.060244	2.528934	0.509240
C	-0.422188	2.003671	1.776467
C	-0.455996	2.864360	2.893787
C	-0.888256	2.389339	4.132774
C	-1.308747	1.058964	4.262191
C	-1.306726	0.204536	3.148929
C	-0.870249	0.674087	1.913483
H	0.181633	-3.030441	-1.515167

```
 H    -0.920597     3.775124    -1.684549
 H    -0.342511     4.848977    -3.849013
 H     1.649491     4.077283    -5.148741
 H     3.075366     2.238712    -4.259415
 H     0.086094     3.628109     0.420341
 H    -0.128971     3.902537     2.786036
 H    -0.902040     3.055307     4.998745
 H    -1.650505     0.689034     5.232430
 H    -1.647342    -0.829001     3.248788
 H    -0.895619     0.033454     1.035636
 H     2.011304    -1.169436     2.298881
 H     1.709830    -2.244855     4.538770
 H    -0.037407    -3.988497     4.870127
 H    -1.508615    -4.703767     2.996314
 C    -1.171919    -1.359973    -1.578803
 C    -0.612160    -0.895356    -2.779615
 C    -1.170102     0.204884    -3.437576
 C    -2.295454     0.840720    -2.902490
 C    -2.864168     0.372062    -1.711719
 C    -2.303260    -0.723785    -1.049079
 H     0.270629    -1.391411    -3.192634
 H    -0.726868     0.564352    -4.369488
 H    -2.735926     1.697003    -3.419257
 H    -3.752093     0.857816    -1.299058
 H    -2.747183    -1.093505    -0.122029
   51
TS AD
 C    -1.760004    -4.464155     2.357710
 C    -0.882948    -4.573809     1.257276
 C     0.551368    -4.487528     1.440184
 C     1.062158    -4.325703     2.750171
 C     0.182014    -4.247215     3.816862
 C    -1.223375    -4.312786     3.626729
 N     1.308666    -4.489109     0.302735
 C     0.646086    -5.118460    -0.738360
 S    -1.339548    -4.592121    -0.399937
Cu     1.232440    -2.527941    -0.165222
 S    -0.984443    -1.992095    -0.684029
 C    -0.565416    -1.724414    -2.371758
 C     0.778858    -1.452126    -2.777428
 C     1.048091    -1.256826    -4.141883
 C     0.021297    -1.288119    -5.084731
 C    -1.301506    -1.529018    -4.685952
 C    -1.588919    -1.745324    -3.341103
 N     1.799699    -1.440637    -1.807776
 C     2.842889    -0.688729    -1.942066
 C     4.003896    -0.708441    -1.064477
 C     4.946938     0.331752    -1.201852
 C     6.074714     0.381534    -0.381071
 C     6.280948    -0.616117     0.578738
 C     5.360067    -1.667850     0.713115
 C     4.232235    -1.717012    -0.101078
 H     0.440518    -6.190683    -0.540347
 H     2.079318    -1.112050    -4.467886
 H     0.255618    -1.133085    -6.140827
 H    -2.104704    -1.551524    -5.426129
 H    -2.614960    -1.935529    -3.017939
 H     2.878430     0.043488    -2.765496
 H     4.782008     1.107561    -1.955100
```

```
 H     6.794257     1.196307    -0.490094
 H     7.165552    -0.582058     1.219879
 H     5.535665    -2.455578     1.449821
 H     3.542631    -2.562891    -0.011225
 H     2.143595    -4.286856     2.894878
 H     0.575602    -4.142330     4.831152
 H    -1.887119    -4.247195     4.491716
 H    -2.840639    -4.507189     2.206458
 C     1.107297    -4.842006    -2.136346
 C     2.448501    -4.482238    -2.350465
 C     2.921403    -4.270465    -3.648023
 C     2.061146    -4.410696    -4.741345
 C     0.724599    -4.771875    -4.533788
 C     0.251772    -4.992584    -3.238860
 H     3.118679    -4.383924    -1.495534
 H     3.969686    -4.001875    -3.803318
 H     2.431206    -4.244240    -5.756194
 H     0.046677    -4.882229    -5.383268
 H    -0.793456    -5.276331    -3.089257
   51
TS D ES
 C     1.875203    -7.755675     1.534629
 C     1.584291    -6.773948     0.574950
 C     1.976341    -5.404637     0.784577
 C     2.649295    -5.037069     1.980972
 C     2.911452    -6.012608     2.921874
 C     2.527826    -7.364066     2.699505
 N     1.680489    -4.565912    -0.220687
 C     1.109101    -5.199083    -1.337666
 S     0.769936    -6.953692    -0.939664
Cu     2.460974    -2.923755    -0.900851
 S     3.436195    -4.010037    -2.894842
 C     2.520894    -2.885329    -3.885765
 C     2.005226    -1.655198    -3.367304
 C     1.202562    -0.844886    -4.187871
 C     0.948511    -1.199210    -5.511898
 C     1.500960    -2.374234    -6.045597
 C     2.280283    -3.199514    -5.242763
 N     2.292339    -1.297148    -2.026281
 C     2.426591    -0.060571    -1.674738
 C     2.670688     0.382615    -0.308130
 C     2.369537     1.721084     0.018789
 C     2.537551     2.187097     1.323702
 C     3.034632     1.329831     2.312843
 C     3.374100     0.006764     1.992616
 C     3.196319    -0.462178     0.693321
 H     2.011873    -5.165196    -2.154297
 H     0.756232     0.061590    -3.774249
 H     0.320063    -0.555218    -6.131805
 H     1.317526    -2.643498    -7.088529
 H     2.713765    -4.116694    -5.647935
 H     2.345197     0.731562    -2.435094
 H     1.985484     2.390111    -0.756715
 H     2.287771     3.221832     1.569897
 H     3.178301     1.697089     3.332140
 H     3.799740    -0.647701     2.757361
 H     3.531687    -1.473969     0.435355
 H     2.935898    -3.993547     2.128029
 H     3.423762    -5.751150     3.850565
```

```
 H     2.751194    -8.112924     3.463317
 H     1.589498    -8.797569     1.375904
 C     0.011302    -4.446337    -2.051518
 C    -0.167700    -4.617024    -3.430534
 C    -1.161340    -3.899802    -4.100680
 C    -1.974532    -3.004716    -3.396243
 C    -1.794561    -2.830430    -2.018567
 C    -0.803388    -3.548209    -1.344500
 H     0.487846    -5.294588    -3.983385
 H    -1.290474    -4.029201    -5.177639
 H    -2.749694    -2.441372    -3.921838
 H    -2.433345    -2.137812    -1.464587
 H    -0.653912    -3.414190    -0.270912
   51
TS D EC
 C     2.895410    -5.438765     2.381991
 C     2.392605    -4.977952     1.157489
 C     1.225908    -4.153111     1.104616
 C     0.562568    -3.795083     2.301023
 C     1.050478    -4.279037     3.502598
 C     2.208365    -5.095406     3.543696
 N     0.862435    -3.757385    -0.141371
 C     1.728559    -4.181963    -1.129104
 S     3.006947    -5.262455    -0.441732
Cu    -0.299453    -2.362611    -0.808654
 S    -1.730277    -1.294291    -2.139697
 C    -0.604734    -0.885596    -3.360582
 C     0.858917    -0.969276    -3.180467
 C     1.712907    -0.603658    -4.278842
 C     1.183406    -0.180850    -5.468486
 C    -0.235429    -0.089474    -5.639358
 C    -1.095808    -0.423540    -4.620461
 N     1.306280    -1.324800    -1.978368
 C     2.570387    -1.639773    -1.637839
 C     2.989796    -1.463842    -0.237154
 C     4.237117    -1.978060     0.170540
 C     4.588748    -1.979143     1.519575
 C     3.700953    -1.465282     2.475063
 C     2.473199    -0.922720     2.074109
 C     2.118722    -0.915981     0.725357
 H     2.341607    -3.078142    -1.418981
 H     2.794673    -0.640957    -4.141586
 H     1.842852     0.106133    -6.291188
 H    -0.637310     0.259819    -6.593908
 H    -2.176455    -0.347734    -4.758696
 H     3.367098    -1.696068    -2.397693
 H     4.919222    -2.395308    -0.575595
 H     5.554503    -2.383920     1.831889
 H     3.975073    -1.472498     3.532993
 H     1.795853    -0.495444     2.817432
 H     1.173729    -0.474566     0.400917
 H    -0.321491    -3.155672     2.251379
 H     0.542259    -4.025636     4.435783
 H     2.571175    -5.461511     4.507178
 H     3.790262    -6.063192     2.423159
 C     1.185621    -4.491735    -2.496932
 C     2.014180    -4.354570    -3.620891
 C     1.505697    -4.590393    -4.899735
 C     0.163223    -4.957507    -5.062160
```

```
 C    -0.663386    -5.099653    -3.942357
 C    -0.155299    -4.871577    -2.659990
 H     3.056509    -4.047715    -3.493604
 H     2.153644    -4.478534    -5.772425
 H    -0.236813    -5.135447    -6.063450
 H    -1.708307    -5.395405    -4.064558
 H    -0.796614    -4.983091    -1.783681
   51
TS D EN
 C     2.607729    -5.358912     2.385960
 C     2.095983    -4.923856     1.154153
 C     0.758058    -4.414290     1.055042
 C    -0.059182    -4.343172     2.212328
 C     0.454240    -4.789343     3.415967
 C     1.778368    -5.297303     3.501710
 N     0.401480    -3.985825    -0.173626
 C     1.428574    -4.063819    -1.120813
 S     2.890593    -4.867345    -0.379737
Cu    -0.859691    -2.683779    -0.758894
 S    -1.566672    -0.953899    -1.835023
 C    -0.447892    -0.948494    -3.203345
 C     0.960559    -1.166879    -3.117991
 C     1.757784    -1.111621    -4.278845
 C     1.194746    -0.821257    -5.515103
 C    -0.186384    -0.571288    -5.607693
 C    -0.984434    -0.619673    -4.471439
 N     1.575332    -1.407414    -1.876316
 C     2.483698    -0.620852    -1.409996
 C     3.129503    -0.820168    -0.119929
 C     4.389163    -0.239601     0.126936
 C     5.020877    -0.442406     1.355024
 C     4.388241    -1.198238     2.351318
 C     3.117002    -1.747147     2.125241
 C     2.490670    -1.557683     0.896941
 H     1.668828    -2.857930    -1.335844
 H     2.828732    -1.304922    -4.186113
 H     1.825872    -0.774629    -6.405634
 H    -0.637397    -0.336116    -6.574821
 H    -2.055587    -0.418027    -4.545362
 H     2.783268     0.262236    -2.000004
 H     4.873621     0.357987    -0.650493
 H     6.003705    -0.003549     1.542534
 H     4.880876    -1.343678     3.316337
 H     2.611856    -2.313070     2.911304
 H     1.483596    -1.932928     0.719802
 H    -1.073483    -3.946510     2.127680
 H    -0.162851    -4.753462     4.316634
 H     2.153385    -5.646972     4.466742
 H     3.627026    -5.742219     2.465105
 C     1.088311    -4.478921    -2.531209
 C     2.053748    -4.312831    -3.535732
 C     1.757662    -4.647970    -4.857020
 C     0.486612    -5.133759    -5.187755
 C    -0.479705    -5.295660    -4.189107
 C    -0.182071    -4.973231    -2.861629
 H     3.039204    -3.910678    -3.281854
 H     2.515278    -4.518850    -5.633611
 H     0.250943    -5.389246    -6.223789
 H    -1.469051    -5.685761    -4.440677
```

```
 H    -0.931240    -5.115369    -2.080093
   51
ES
 C    -0.959726    -4.659774     2.215941
 C    -0.871555    -3.756448     1.148423
 C    -0.767714    -2.363797     1.369447
 C    -0.766099    -1.855791     2.678210
 C    -0.856809    -2.752124     3.738438
 C    -0.948535    -4.141387     3.510281
 N    -0.677368    -1.611030     0.202494
 C    -0.743017    -2.360293    -0.881640
 S    -0.892714    -4.071268    -0.573711
Cu    -0.146639     0.260678     0.136637
 S     1.658902     0.887170    -1.914733
 C     0.516215     2.239932    -2.189593
 C    -0.161100     2.799197    -1.084016
 C    -1.043764     3.875226    -1.281796
 C    -1.245309     4.397518    -2.558979
 C    -0.562668     3.849941    -3.653319
 C     0.319340     2.783572    -3.466358
 N     0.033236     2.221594     0.203376
 C     0.201660     2.994365     1.226770
 C     0.423615     2.548941     2.596551
 C     0.162769     3.462247     3.639191
 C     0.340130     3.085112     4.971105
 C     0.807537     1.800866     5.276195
 C     1.104785     0.896182     4.246123
 C     0.917173     1.266878     2.916060
 H     1.308922     0.178147    -3.016255
 H    -1.593695     4.275806    -0.426990
 H    -1.940773     5.227774    -2.702209
 H    -0.712932     4.258505    -4.655523
 H     0.864296     2.366769    -4.316244
 H     0.183533     4.084616     1.070844
 H    -0.193393     4.467949     3.397592
 H     0.121982     3.794689     5.772741
 H     0.959559     1.509178     6.318614
 H     1.498269    -0.095506     4.482688
 H     1.197389     0.574049     2.117872
 H    -0.701746    -0.779799     2.844101
 H    -0.862656    -2.374608     4.763793
 H    -1.018819    -4.823891     4.360511
 H    -1.039510    -5.735130     2.042265
 C    -0.717240    -1.814823    -2.244592
 C     0.045890    -2.425416    -3.255929
 C     0.109567    -1.846767    -4.526483
 C    -0.600956    -0.669862    -4.800750
 C    -1.384687    -0.074502    -3.803639
 C    -1.442630    -0.642118    -2.531145
 H     0.613617    -3.333304    -3.036573
 H     0.717266    -2.314116    -5.305036
 H    -0.550950    -0.222566    -5.796871
 H    -1.946817     0.836896    -4.016556
 H    -2.057471    -0.184846    -1.751905
   51
EC
 C    -1.599478    -1.252931     4.831664
 C    -0.998647    -1.439795     3.579756
 C    -1.235191    -0.546695     2.510845
```

```
 C    -2.080322     0.560913     2.687899
 C    -2.677546     0.746849     3.930431
 C    -2.439651    -0.151746     4.992207
 N    -0.551482    -0.864370     1.345281
 C     0.184142    -1.950382     1.469388
 S     0.092660    -2.700325     3.048292
Cu    -0.450744     0.402424    -0.168546
 S    -2.399512     1.016223    -1.370503
 C    -1.581186     1.392712    -2.794857
 C    -0.113747     1.636355    -2.765990
 C     0.489102     2.354844    -3.866246
 C    -0.245699     2.601258    -4.992070
 C    -1.626669     2.204478    -5.082884
 C    -2.270293     1.600714    -4.030056
 N     0.541341     1.091848    -1.769770
 C     1.932488     1.399687    -1.446293
 C     2.020771     1.287607     0.063008
 C     2.774407     0.285509     0.686634
 C     2.726313     0.133603     2.075876
 C     1.916184     0.969705     2.854081
 C     1.159337     1.973966     2.242668
 C     1.209577     2.135057     0.852270
 H     2.587036     0.649983    -1.924354
 H     1.547166     2.617727    -3.821013
 H     0.221815     3.087550    -5.852030
 H    -2.176582     2.414515    -6.003932
 H    -3.329936     1.342660    -4.088866
 H     2.237862     2.401705    -1.795805
 H     3.379411    -0.392941     0.080490
 H     3.316412    -0.651787     2.554223
 H     1.875018     0.838295     3.937981
 H     0.528227     2.630711     2.845646
 H     0.638016     2.935804     0.373104
 H    -2.254028     1.249133     1.857559
 H    -3.342934     1.598814     4.088435
 H    -2.922747     0.016320     5.957690
 H    -1.418806    -1.946504     5.655761
 C     1.026344    -2.500314     0.401864
 C     2.257803    -3.113044     0.702827
 C     3.087269    -3.568885    -0.323075
 C     2.695870    -3.423727    -1.660510
 C     1.462057    -2.835972    -1.966993
 C     0.627824    -2.382341    -0.943994
 H     2.578976    -3.204236     1.743429
 H     4.045050    -4.034802    -0.079148
 H     3.346486    -3.782096    -2.462343
 H     1.139441    -2.747586    -3.007479
 H    -0.351845    -1.964094    -1.185797
   51
EN
 C     0.377747    -1.879620     4.793357
 C     0.578896    -1.663137     3.423916
 C    -0.508597    -1.562229     2.528083
 C    -1.827500    -1.664843     3.001965
 C    -2.028702    -1.874877     4.362400
 C    -0.936065    -1.983211     5.249269
 N    -0.139000    -1.331520     1.209306
 C     1.169061    -1.245660     1.057467
 S     2.074670    -1.473725     2.539522
```

```
Cu    -1.486261    -0.908729    -0.132274
 S    -2.930040    -0.138036    -1.594178
 C    -1.869894     0.383552    -2.926259
 C    -0.765638     1.253153    -2.721450
 C     0.062227     1.678194    -3.770513
 C    -0.205017     1.246916    -5.065552
 C    -1.301750     0.398338    -5.299955
 C    -2.120911    -0.021675    -4.251384
 N    -0.541975     1.658956    -1.390976
 C     0.579667     1.934339    -0.790027
 C     0.707560     2.141304     0.630599
 C     1.973149     2.521542     1.130716
 C     2.181258     2.636867     2.503494
 C     1.135583     2.353539     3.391975
 C    -0.124775     1.968254     2.907770
 C    -0.345347     1.872880     1.537977
 H    -1.404313     1.554441    -0.829690
 H     0.891255     2.360647    -3.569994
 H     0.422612     1.580840    -5.894619
 H    -1.520735     0.064430    -6.317420
 H    -2.966490    -0.685728    -4.443451
 H     1.483829     1.935297    -1.407140
 H     2.788037     2.716639     0.429621
 H     3.158851     2.939814     2.885348
 H     1.301104     2.430910     4.469594
 H    -0.933357     1.737961     3.604909
 H    -1.327427     1.550642     1.182300
 H    -2.666529    -1.581358     2.305945
 H    -3.046163    -1.961935     4.750526
 H    -1.121740    -2.153420     6.312421
 H     1.219941    -1.965696     5.483330
 C     1.840161    -0.941565    -0.212985
 C     3.085726    -0.281494    -0.226407
 C     3.680607     0.082214    -1.436238
 C     3.041541    -0.203781    -2.650039
 C     1.815607    -0.880825    -2.648993
 C     1.226649    -1.259324    -1.442460
 H     3.575278    -0.022741     0.715113
 H     4.645847     0.594790    -1.431875
 H     3.504710     0.087848    -3.595981
 H     1.317808    -1.121376    -3.590503
 H     0.292971    -1.827343    -1.457914
   51
ECu
 C    -0.464142     2.471710    -4.172586
 C    -0.242845     1.814304    -2.949226
 C     0.412464     2.512644    -1.912061
 C     0.766639     3.864366    -2.073002
 C     0.524015     4.504953    -3.285343
 C    -0.077504     3.800865    -4.340001
 S    -0.803979     0.154455    -2.695743
Cu    -0.447456     0.240305    -0.464994
 N     0.691957     1.774003    -0.712829
 C     1.669051     2.113311     0.073129
 C     2.093252     1.479127     1.310110
 C     2.015093     0.088351     1.548777
 C     2.422381    -0.435740     2.776801
 C     2.914103     0.413073     3.775733
 C     3.031060     1.789801     3.536026
```

```
 C     2.645527     2.317012     2.304486
 H    -0.320255     0.418502     1.001985
 H     1.205331     4.428354    -1.247519
 H     0.789623     5.557654    -3.404136
 H    -0.266636     4.301329    -5.293015
 H    -0.958051     1.933492    -4.985143
 H     2.248462     3.002157    -0.211582
 H     2.744303     3.389345     2.113864
 H     3.431704     2.449539     4.309188
 H     3.231381    -0.000614     4.736379
 H     2.374782    -1.514596     2.938086
 H     1.713840    -0.594698     0.756490
 N    -1.603596    -1.231670    -0.023915
 C    -1.199615    -2.427254     0.358916
 S    -2.503066    -3.473680     0.847009
 C    -3.659678    -2.197057     0.523662
 C    -2.981731    -1.056113     0.041676
 C    -3.689892     0.103241    -0.309054
 C    -5.073079     0.094419    -0.162681
 C    -5.747300    -1.046390     0.322483
 C    -5.052921    -2.204630     0.668951
 H    -5.579086    -3.087451     1.038309
 H    -6.834747    -1.024822     0.424733
 H    -5.648434     0.982614    -0.433432
 H    -3.158333     0.969500    -0.708523
 C     0.200095    -2.865333     0.361988
 C     1.039303    -2.531028    -0.720700
 C     2.379165    -2.923615    -0.708708
 C     2.889477    -3.655565     0.370923
 C     2.053272    -4.005937     1.438970
 C     0.711790    -3.617921     1.436237
 H     0.062189    -3.878641     2.275818
 H     2.448505    -4.583322     2.278372
 H     3.938245    -3.962937     0.375752
 H     3.024015    -2.668126    -1.553051
 H     0.641321    -1.981283    -1.577607
   51
ENR
 C     2.293368    -1.844193     2.253270
 C     2.101130    -2.451619     0.996138
 C     3.199424    -3.040034     0.341459
 C     4.468238    -3.000638     0.922748
 C     4.654622    -2.378592     2.163529
 C     3.563631    -1.805000     2.829219
 C     0.775200    -2.435470     0.371519
 N    -0.096609    -1.460212     0.528440
 C    -1.267340    -1.665340    -0.190918
 C    -1.279126    -2.865230    -0.936197
 S     0.223330    -3.724829    -0.673339
 C    -2.362207    -0.786372    -0.244742
 C    -3.450960    -1.134539    -1.037393
 C    -3.458824    -2.337758    -1.774722
 C    -2.376040    -3.215884    -1.734514
Cu     0.311157     0.298164     1.247537
 S     0.259760     2.497434     1.786577
 C    -1.453640     2.705732     1.289550
 C    -1.575971     3.435624     0.091032
 N    -0.358999     3.862841    -0.486177
 C     0.769685     3.127765    -0.031338
```

```
 C    -2.576622     2.247186     1.978126
 C    -3.845520     2.523443     1.450393
 C    -3.975790     3.247948     0.258541
 C    -2.843877     3.702063    -0.430245
 C     1.107665     1.883983    -0.818446
 C     2.345764     1.249527    -0.594723
 C     2.652721     0.055278    -1.248671
 C     1.728497    -0.514549    -2.134834
 C     0.506781     0.120939    -2.372944
 C     0.196652     1.321788    -1.724664
 H    -2.937492     4.255354    -1.367437
 H    -4.969634     3.458628    -0.143434
 H    -4.735244     2.172904     1.978534
 H    -2.473073     1.687851     2.910738
 H     1.649802     3.770350     0.108297
 H     3.065095     1.691865     0.101259
 H     3.611600    -0.434100    -1.064907
 H     1.964673    -1.452889    -2.642343
 H    -0.214050    -0.318290    -3.066467
 H    -0.752128     1.823615    -1.917987
 H    -2.349088     0.146479     0.323831
 H    -4.313401    -0.466087    -1.089717
 H    -4.327436    -2.588226    -2.388292
 H    -2.385672    -4.145855    -2.307069
 H    -0.234175     4.872474    -0.498394
 H     1.434281    -1.441268     2.796722
 H     3.701087    -1.342278     3.809673
 H     5.648479    -2.350316     2.617295
 H     5.316332    -3.453674     0.403565
 H     3.063948    -3.505992    -0.638077
   51
TS B BT
 C     4.911212    -1.883907    -3.771398
 C     3.750862    -2.622362    -3.452673
 C     3.175220    -3.466384    -4.429027
 C     3.733354    -3.545072    -5.700846
 C     4.870575    -2.784307    -6.015254
 C     5.460740    -1.956612    -5.050139
 C     3.213557    -2.525586    -2.114123
 N     2.019477    -2.921603    -1.775684
 C     1.675304    -3.066695    -0.434769
 C     0.300334    -2.892810    -0.028965
 C    -0.033794    -3.017233     1.349845
 C     0.929465    -3.337065     2.290693
 C     2.263812    -3.549173     1.880553
 C     2.625263    -3.424825     0.541401
 S    -0.957874    -2.545938    -1.155855
Cu     0.367512    -2.476822    -3.035352
 S     0.464899    -1.755487    -5.174941
 C     0.944187     0.321146    -1.714266
 N     0.700422     0.356157    -2.970271
 C    -0.560843     0.241851    -3.504298
 C    -0.804867    -0.746795    -4.550550
 C    -2.119449    -0.822071    -5.106585
 C    -3.129123     0.017871    -4.679684
 C    -2.872882     0.978357    -3.670053
 C    -1.610612     1.089711    -3.096437
 H     0.131300     0.111061    -0.991590
 H     3.654608    -3.622532     0.237951
```

```
 H     3.023054   -3.820480    2.618684
 H     0.656062   -3.441268    3.343094
 H    -1.074180   -2.865964    1.646563
 H    -1.408699    1.842412   -2.331498
 H    -3.677804    1.636721   -3.332748
 H    -4.125192   -0.052113   -5.122879
 H    -2.299807   -1.564839   -5.886664
 C     2.287563    0.446847   -1.155688
 H     3.870690   -2.080378   -1.349942
 H     2.304638   -4.071756   -4.168838
 H     3.291402   -4.203673   -6.452191
 H     5.305798   -2.847575   -7.016070
 H     6.352135   -1.375676   -5.298371
 H     5.360406   -1.244114   -3.008445
 C     2.488659    0.141917    0.203380
 C     3.772133    0.190596    0.751933
 C     4.858387    0.561787   -0.050818
 C     4.661789    0.876663   -1.405279
 C     3.385688    0.811251   -1.961094
 H     1.635197   -0.148683    0.822904
 H     3.926691   -0.052075    1.806117
 H     5.861573    0.614274    0.380643
 H     5.511952    1.176067   -2.023616
 H     3.212055    1.030180   -3.017123
   51
BT
 C     4.734811   -1.898124   -3.256617
 C     3.588713   -2.713323   -3.143628
 C     3.142145   -3.453705   -4.259614
 C     3.817560   -3.354421   -5.475569
 C     4.933241   -2.513308   -5.589695
 C     5.390544   -1.785576   -4.481354
 C     2.923062   -2.793285   -1.859367
 N     1.650721   -2.996999   -1.679538
 C     1.148772   -3.281229   -0.392285
 C    -0.179747   -2.876798   -0.079594
 C    -0.651183   -3.056593    1.237886
 C     0.140291   -3.685235    2.194721
 C     1.429281   -4.140421    1.864154
 C     1.926849   -3.943202    0.580038
 S    -1.248571   -2.198561   -1.301922
Cu     0.262009   -2.259607   -2.957601
 S     0.928171   -1.404468   -4.925852
 C     1.369373    0.348966   -1.796621
 N     0.715310    0.818619   -2.784630
 C    -0.459248    0.434368   -3.299607
 C    -0.513239   -0.752575   -4.191791
 C    -1.818416   -1.144594   -4.691404
 C    -2.940793   -0.418282   -4.401026
 C    -2.844784    0.756463   -3.591498
 C    -1.643029    1.183967   -3.069045
 H     0.848761   -0.369239   -1.131894
 H     2.915692   -4.322066    0.312662
 H     2.039401   -4.654898    2.610066
 H    -0.252459   -3.841400    3.202417
 H    -1.659572   -2.720252    1.490241
 H    -1.579008    2.075422   -2.442844
 H    -3.753221    1.322525   -3.367943
 H    -3.911629   -0.720416   -4.799611
```

```
 H    -1.860164    -2.025720    -5.335259
 C     2.757473     0.644747    -1.480496
 H     3.558065    -2.651033    -0.972682
 H     2.283339    -4.119037    -4.154122
 H     3.480526    -3.937437    -6.335874
 H     5.458395    -2.435344    -6.545188
 H     6.263805    -1.135863    -4.575552
 H     5.081999    -1.333434    -2.387650
 C     3.307231     0.083958    -0.310793
 C     4.653222     0.291102    -0.002616
 C     5.451710     1.057447    -0.862545
 C     4.908342     1.615322    -2.031206
 C     3.566319     1.409939    -2.343878
 H     2.671073    -0.512416     0.350557
 H     5.080674    -0.136398     0.907562
 H     6.504999     1.223103    -0.621256
 H     5.539379     2.210396    -2.695859
 H     3.126674     1.821892    -3.255074
   51
TS BT DS
 C     5.096390    -3.691866    -2.194691
 C     3.709013    -3.780894    -2.436868
 C     3.216555    -3.531271    -3.736530
 C     4.089983    -3.172042    -4.758693
 C     5.465146    -3.064526    -4.501709
 C     5.968265    -3.327109    -3.221539
 C     2.840082    -4.177925    -1.340089
 N     1.557016    -3.994853    -1.306729
 C     0.785892    -4.595505    -0.301144
 C    -0.377429    -3.905068     0.193697
 C    -1.141736    -4.504212     1.231853
 C    -0.807963    -5.754049     1.731140
 C     0.309161    -6.438981     1.214186
 C     1.092063    -5.867428     0.208921
 S    -0.863208    -2.371498    -0.436844
Cu     0.566396    -2.374635    -2.228065
 S     0.877469    -1.057852    -4.036487
 C    -0.466044     0.022824    -3.697966
 C    -0.139870     1.227506    -2.939339
 C    -1.180986     2.159916    -2.631113
 C    -2.472051     1.914917    -3.052206
 C    -2.774748     0.749926    -3.799469
 C    -1.782498    -0.182478    -4.120285
 N     1.118513     1.438081    -2.592324
 C     2.080115     0.512817    -2.704933
 H     2.143694    -0.210539    -1.873181
 H     1.937819    -6.422025    -0.202971
 H     0.567916    -7.428986     1.598176
 H    -1.413810    -6.209531     2.517678
 H    -2.007438    -3.962139     1.619292
 H    -0.917131     3.053032    -2.061739
 H    -3.267848     2.624364    -2.813346
 H    -3.799931     0.577248    -4.136651
 H    -2.034610    -1.072686    -4.700106
 C     3.359697     0.811226    -3.358354
 H     3.336896    -4.661785    -0.482042
 H     2.151790    -3.651892    -3.940155
 H     3.704352    -2.983500    -5.763095
 H     6.146883    -2.782013    -5.307681
```

```
 H     7.041075   -3.254865   -3.026980
 H     5.484183   -3.908753   -1.195091
 C     4.453409   -0.050619   -3.159801
 C     5.679158    0.229062   -3.763493
 C     5.818860    1.364114   -4.572347
 C     4.729153    2.222285   -4.778617
 C     3.502897    1.949866   -4.174667
 H     4.338105   -0.944781   -2.540761
 H     6.527775   -0.438633   -3.601806
 H     6.781510    1.584555   -5.041009
 H     4.842737    3.109839   -5.405890
 H     2.650918    2.619739   -4.310880
   51
DS
 C     5.068566   -2.993103   -1.468276
 C     3.758391   -3.228802   -1.938366
 C     3.458310   -2.979487   -3.296344
 C     4.437290   -2.481527   -4.150180
 C     5.731795   -2.233503   -3.666691
 C     6.047632   -2.491883   -2.327664
 C     2.786046   -3.786770   -1.012483
 N     1.502648   -3.818223   -1.205215
 C     0.680538   -4.584194   -0.365467
 C    -0.683973   -4.169483   -0.150325
 C    -1.505454   -4.930980    0.726889
 C    -1.027972   -6.084488    1.329184
 C     0.291209   -6.508528    1.076312
 C     1.129078   -5.770916    0.236715
 S    -1.361305   -2.790464   -0.935688
Cu     0.456032   -2.315142   -2.241651
 S     0.990042   -0.599494   -3.634220
 C     1.804752    0.578825   -2.184067
 N     0.787818    1.446245   -1.784307
 C    -0.375227    1.334643   -2.407274
 C    -0.505532    0.323379   -3.438448
 C    -1.690356    0.167285   -4.145146
 C    -2.778219    1.002119   -3.836468
 C    -2.680867    1.988313   -2.828184
 C    -1.505437    2.162246   -2.118351
 H     2.053529   -0.150834   -1.393893
 H     2.137401   -6.133752    0.028288
 H     0.666951   -7.425994    1.536268
 H    -1.674868   -6.667232    1.988749
 H    -2.528678   -4.592048    0.904322
 H    -1.403403    2.920422   -1.339635
 H    -3.544903    2.621091   -2.611853
 H    -3.713376    0.886255   -4.389851
 H    -1.782698   -0.589568   -4.927168
 C     3.050550    1.216285   -2.724162
 H     3.202257   -4.212692   -0.084134
 H     2.463517   -3.212069   -3.679287
 H     4.200853   -2.293308   -5.199876
 H     6.496702   -1.842918   -4.342243
 H     7.057992   -2.306943   -1.955641
 H     5.311834   -3.206069   -0.423302
 C     4.285815    0.587982   -2.517748
 C     5.455432    1.156971   -3.028214
 C     5.393518    2.355603   -3.747566
 C     4.158556    2.985457   -3.954491
```

```
 C     2.988889     2.419775    -3.443854
 H     4.330429    -0.349401    -1.957983
 H     6.416609     0.665782    -2.858826
 H     6.308267     2.804757    -4.142952
 H     4.110478     3.925482    -4.509867
 H     2.025436     2.913855    -3.589693
   51
TS DS ESS
 C     5.059348    -3.324482    -3.642575
 C     3.706981    -3.613593    -3.368669
 C     2.811615    -3.806081    -4.445253
 C     3.255877    -3.674983    -5.758517
 C     4.597449    -3.353497    -6.017577
 C     5.498879    -3.183116    -4.959824
 C     3.284781    -3.702635    -1.978849
 N     2.054516    -3.570014    -1.592995
 C     1.672083    -3.774557    -0.252897
 C     0.497670    -3.116060     0.248906
 C     0.152518    -3.286714     1.612212
 C     0.899607    -4.109045     2.447211
 C     2.014582    -4.793108     1.935789
 C     2.388614    -4.630465     0.601332
 S    -0.580923    -2.171260    -0.754713
Cu     0.729136    -2.437629    -2.676660
 S     1.227303    -0.365679    -3.580135
 C     0.831239     0.550265    -1.877825
 N    -0.136539     1.485317    -2.135510
 C    -0.773580     1.329292    -3.291186
 C    -0.250576     0.331201    -4.206366
 C    -0.879447     0.079496    -5.422608
 C    -2.022111     0.821559    -5.749483
 C    -2.541165     1.810321    -4.878595
 C    -1.933597     2.071700    -3.664503
 H     0.320632    -0.324097    -1.298188
 H     3.238013    -5.194594     0.210706
 H     2.591018    -5.462899     2.578639
 H     0.607922    -4.235538     3.492319
 H    -0.729676    -2.767254     1.992933
 H    -2.314750     2.823724    -2.970970
 H    -3.433898     2.366664    -5.173310
 H    -2.520093     0.636377    -6.704756
 H    -0.488751    -0.668227    -6.115999
 C     2.072614     0.924097    -1.134518
 H     4.083787    -3.858481    -1.235890
 H     1.781505    -4.116268    -4.243825
 H     2.565584    -3.844234    -6.588712
 H     4.943409    -3.254083    -7.049628
 H     6.545685    -2.945908    -5.164021
 H     5.760502    -3.195959    -2.812807
 C     2.845191    -0.097910    -0.558914
 C     4.020659     0.216953     0.124322
 C     4.423141     1.554175     0.241489
 C     3.647727     2.573182    -0.325070
 C     2.471764     2.262333    -1.014095
 H     2.513101    -1.134929    -0.647040
 H     4.619421    -0.577068     0.577842
 H     5.340738     1.802847     0.780731
 H     3.960542     3.616004    -0.229298
 H     1.852794     3.047861    -1.452909
```

```
  51
ESS
 C     2.032532   -3.128056   -2.265755
 C     0.873425   -2.392058   -1.951151
 C     0.428912   -1.393341   -2.842764
 C     1.157034   -1.106033   -3.994596
 C     2.334814   -1.816160   -4.276694
 C     2.766800   -2.832429   -3.415908
 C     0.183649   -2.701097   -0.704778
 N    -0.599773   -1.888354   -0.069986
 C    -1.303252   -2.343979    1.074612
 C    -1.534007   -1.462957    2.159862
 C    -2.248860   -1.899187    3.280531
 C    -2.743777   -3.205965    3.339866
 C    -2.528761   -4.078352    2.268225
 C    -1.819371   -3.650352    1.144606
 S    -0.995731    0.258816    2.110262
Cu    -0.560607    0.122784   -0.303875
 S     0.106084    2.077741   -1.339149
 C     1.190387    2.139234    0.153433
 N     0.780159    2.966276    1.045067
 C    -0.378745    3.631735    0.696526
 C    -0.929454    3.280044   -0.564009
 C    -2.094977    3.872332   -1.052265
 C    -2.725108    4.826511   -0.246987
 C    -2.196103    5.182311    1.007664
 C    -1.026481    4.594379    1.486839
 H     0.337371    0.072834    2.302415
 H    -1.692079   -4.321227    0.292322
 H    -2.928807   -5.094746    2.297645
 H    -3.304651   -3.535357    4.217434
 H    -2.415082   -1.208321    4.110125
 H    -0.599839    4.865044    2.454578
 H    -2.708568    5.934603    1.611821
 H    -3.640658    5.304693   -0.603176
 H    -2.505264    3.606219   -2.028754
 C     2.314401    1.206654    0.285539
 H     0.385162   -3.695861   -0.275350
 H    -0.505903   -0.864096   -2.643054
 H     0.802761   -0.338812   -4.687558
 H     2.904314   -1.588969   -5.181642
 H     3.672591   -3.398472   -3.646507
 H     2.365597   -3.921490   -1.590498
 C     2.739756    0.395219   -0.783537
 C     3.780759   -0.517471   -0.601642
 C     4.406428   -0.630374    0.645366
 C     3.990508    0.177967    1.713192
 C     2.952792    1.093515    1.538717
 H     2.267209    0.472681   -1.765546
 H     4.101109   -1.137353   -1.440995
 H     5.223105   -1.343048    0.785660
 H     4.483028    0.096020    2.685327
 H     2.622375    1.737287    2.356530
  51
TS B ESS
 C     4.937306   -2.055590   -3.566935
 C     3.778215   -2.782070   -3.223984
 C     3.066277   -3.461115   -4.235140
 C     3.483982   -3.380765   -5.560587
```

```
 C     4.620816    -2.628329    -5.895040
 C     5.350517    -1.970061    -4.897052
 C     3.382030    -2.821447    -1.824765
 N     2.198740    -3.133768    -1.395635
 C     1.988445    -3.288838    -0.007029
 C     0.723085    -2.964430     0.553373
 C     0.510134    -3.114215     1.934048
 C     1.526612    -3.589519     2.764692
 C     2.766359    -3.934407     2.212409
 C     2.990853    -3.791837     0.841702
 S    -0.617393    -2.387010    -0.458916
Cu     0.511700    -2.689393    -2.525862
 S    -0.068196    -2.030031    -4.559072
 C     0.477520     0.093179    -1.543864
 N    -0.155979     0.420089    -2.532257
 C    -0.969367     0.473692    -3.564918
 C    -0.996944    -0.593943    -4.570845
 C    -1.840831    -0.356930    -5.699917
 C    -2.615734     0.775610    -5.814546
 C    -2.601018     1.788805    -4.808685
 C    -1.791650     1.647817    -3.715030
 H    -0.151280    -0.876561    -0.764594
 H     3.945316    -4.106422     0.415027
 H     3.558776    -4.335837     2.848991
 H     1.344882    -3.710194     3.835164
 H    -0.468033    -2.858757     2.348094
 H    -1.744517     2.408511    -2.933074
 H    -3.230219     2.675039    -4.916758
 H    -3.258780     0.898387    -6.689859
 H    -1.872629    -1.124311    -6.476430
 C     1.860526     0.274910    -1.129256
 H     4.162558    -2.539384    -1.099312
 H     2.200987    -4.071359    -3.968028
 H     2.932410    -3.913903    -6.338465
 H     4.946945    -2.569638    -6.936771
 H     6.244920    -1.399178    -5.158091
 H     5.502321    -1.549757    -2.779674
 C     2.233401    -0.043146     0.190407
 C     3.567539     0.081400     0.579397
 C     4.525489     0.518809    -0.344634
 C     4.155655     0.834545    -1.661765
 C     2.826975     0.712778    -2.060353
 H     1.479599    -0.387746     0.899999
 H     3.860684    -0.162380     1.602825
 H     5.569785     0.618685    -0.036797
 H     4.908355     1.175039    -2.376560
 H     2.525701     0.937967    -3.085890
   51
I
 C     2.286976    -2.450642     1.628301
 C     2.115432    -1.053668     1.755384
 C     1.796129    -0.515450     3.016592
 C     1.616737    -1.356534     4.117679
 C     1.766154    -2.740602     3.973643
 C     2.108784    -3.287788     2.726720
 C     2.212857    -0.148161     0.615880
 N     2.144882    -0.568215    -0.604056
 C     2.219528     0.301647    -1.710403
 C     1.494692    -0.027558    -2.901498
```

```
 C     1.538089     0.879279    -3.981806
 C     2.284764     2.054228    -3.912068
 C     3.024912     2.347438    -2.757432
 C     2.992941     1.473439    -1.671760
 S     0.512234    -1.494354    -3.098750
 S    -1.824558     0.097555    -2.000916
 C    -3.261534    -0.699194    -1.550524
 C    -3.234925    -1.103549    -0.138302
 N    -2.171184    -0.782682     0.550502
 C    -1.185724    -0.103143    -0.197911
 C    -4.372246    -1.806879     0.396869
 C    -5.441478    -2.072279    -0.421422
 C    -5.446272    -1.665488    -1.795101
 C    -4.373646    -0.993135    -2.362460
 C    -0.698282     1.200164     0.412633
 C    -0.009708     2.149613    -0.358969
 C     0.532255     3.288377     0.243378
 C     0.386775     3.493592     1.620361
 C    -0.309625     2.554542     2.389945
 C    -0.850353     1.411649     1.792353
 H     0.113655     2.008557    -1.434439
 H     1.064185     4.019084    -0.370564
 H     0.804054     4.388330     2.089333
 H    -0.437572     2.713043     3.464058
 H    -1.382968     0.670473     2.389482
 H    -4.392986    -0.693856    -3.412337
 H    -6.320622    -1.891693    -2.410530
 H    -6.311176    -2.603270    -0.027041
 H    -4.348807    -2.108722     1.445507
 H    -0.322231    -0.775635    -0.346181
 H     0.977425     0.639060    -4.888261
 H     2.306137     2.734036    -4.767215
 H     3.635002     3.252645    -2.708521
 H     3.583805     1.691126    -0.779530
 H     2.274299     0.928813     0.833098
 H     1.665038     0.564835     3.116478
 H     1.360455    -0.932664     5.091619
 H     1.630902    -3.397626     4.836486
 H     2.256907    -4.365612     2.624362
 H     2.634562    -2.872923     0.675403
Cu     1.355330    -2.350206    -1.198068
   51
II
   C   1.610741  -2.282935   1.257294
   C   1.733144  -0.919777   1.671497
   C   1.223159  -0.531586   2.923020
   C   0.567133  -1.459405   3.738823
   C   0.388214  -2.780116   3.309908
   C   0.916494  -3.195794   2.077030
   C   2.307488   0.077446   0.745035
   N   2.475214  -0.263974  -0.471993
   C   2.904917   0.558441  -1.488884
   C   2.229845   0.426232  -2.756171
   C   2.656607   1.252911  -3.833239
   C   3.709128   2.144882  -3.677678
   C   4.364188   2.253044  -2.433942
   C   3.961688   1.471376  -1.348634
   S   0.916866  -0.666857  -2.960402
   S  -3.518836   0.946082  -1.306275
```

```
   C  -4.097488  -0.569307  -0.686557
   C  -3.009731  -1.402660  -0.235711
   N  -1.780739  -0.896183  -0.391286
   C  -1.747451   0.383992  -1.060514
   C  -3.295837  -2.673935   0.338835
   C  -4.610630  -3.083423   0.444351
   C  -5.671642  -2.254909  -0.009846
   C  -5.423369  -1.002832  -0.572823
   C  -0.895425   1.408123  -0.342335
   C  -0.040043   2.244658  -1.070462
   C   0.752769   3.188117  -0.408974
   C   0.685592   3.304001   0.983890
   C  -0.175542   2.472863   1.714248
   C  -0.961683   1.526263   1.054617
   H   0.014897   2.148189  -2.156937
   H   1.423297   3.830805  -0.984053
   H   1.296816   4.047756   1.501745
   H  -0.239192   2.571092   2.801162
   H  -1.632371   0.873353   1.619098
   H  -6.246428  -0.372795  -0.916723
   H  -6.702373  -2.605301   0.083949
   H  -4.843915  -4.058775   0.877778
   H  -2.466683  -3.298963   0.679025
   H  -1.338145   0.235176  -2.082591
   H   2.133920   1.166099  -4.788632
   H   4.030842   2.763177  -4.519035
   H   5.193261   2.955586  -2.315386
   H   4.478198   1.545115  -0.388726
   H   2.456393   1.106433   1.117729
   H   1.325811   0.508763   3.239065
   H   0.176647  -1.146248   4.710344
   H  -0.139171  -3.495552   3.945188
   H   0.835361  -4.241540   1.769877
   H   2.160014  -2.620603   0.371856
  Cu  -0.091955  -1.586504   0.232443
  27
FS
 C     2.081793    -0.278756     2.270705
 C     0.836059    -0.086447     1.645545
 C    -0.306464     0.137798     2.459422
 C    -0.184018     0.197349     3.850778
 C     1.063773     0.002903     4.451030
 C     2.194740    -0.234842     3.659011
 N     0.647903    -0.130216     0.259456
 C     1.546722    -0.055051    -0.659846
 C     1.101721    -0.097788    -2.057319
 C    -0.132634    -0.723464    -2.397487
 C    -0.649933    -0.606153    -3.689832
 C     0.050439     0.130393    -4.658445
 C     1.284930     0.706603    -4.342689
 C     1.814624     0.587635    -3.050465
 S    -1.952846     0.439967     1.732898
 H    -1.062857     0.398490     4.468023
 H     1.151377     0.041286     5.539294
 H     3.169243    -0.389850     4.128079
 H     2.963394    -0.482994     1.658984
 H    -2.548832    -0.706066     2.152729
 H     2.614042     0.108629    -0.442340
 H     2.767865     1.062519    -2.802321
```

```
 H     1.838858     1.260251    -5.104673
 H    -0.355729     0.226228    -5.668269
 H    -1.577273    -1.119355    -3.956481
 H    -0.573016    -1.481062    -1.721402
Cu    -1.307869    -0.105046    -0.432886
   27
FS'
 C     2.519585     0.713542     1.356059
 C     1.309812     0.108005     0.973171
 C     0.515955    -0.518081     1.972827
 C     0.934536    -0.528015     3.306173
 C     2.149736     0.067387     3.662390
 C     2.938217     0.688245     2.686201
 N     0.822325     0.109499    -0.339378
 C     1.474562     0.376139    -1.417571
 C     0.757633     0.297944    -2.694619
 C    -0.657317     0.455604    -2.735587
 C    -1.360556     0.209105    -3.916688
 C    -0.668849    -0.194576    -5.070064
 C     0.725019    -0.306791    -5.047867
 C     1.438569    -0.053932    -3.868471
 S    -1.098807    -1.280502     1.598010
 H     0.311240    -1.001674     4.068073
 H     2.472676     0.054301     4.705913
 H     3.879903     1.166735     2.965701
 H     3.126468     1.224377     0.605136
 H    -0.663352    -2.538184     1.318981
 H     2.554474     0.593010    -1.424822
 H     2.526109    -0.166002    -3.850313
 H     1.262872    -0.598900    -5.953073
 H    -1.218740    -0.390483    -5.993742
 H    -2.441124     0.368284    -3.953251
 H    -1.180186     0.979565    -1.912501
Cu    -1.120107    -0.559542    -0.619950
   27
FC
 C     2.051346    -0.452194     2.326251
 C     1.041283     0.056516     1.507441
 C    -0.200062     0.439734     2.092998
 C    -0.407603     0.283071     3.479135
 C     0.613248    -0.242142     4.281571
 C     1.843284    -0.583697     3.707656
 C     1.125566     0.007356    -0.007366
 N     0.086214    -0.949733    -0.386027
Cu    -1.048594    -1.455164     1.296854
 S    -2.504196    -2.462565    -0.194871
 C    -1.755121    -1.868157    -1.581841
 C    -0.581972    -0.930905    -1.501664
 C    -0.230044    -0.156695    -2.677412
 C    -0.814755    -0.446751    -3.873439
 C    -1.828332    -1.471966    -3.977732
 C    -2.275337    -2.165056    -2.880995
 H    -3.074361    -2.904158    -2.971475
 H    -2.265236    -1.678539    -4.958343
 H    -0.507756     0.084555    -4.777830
 H     0.562588     0.589597    -2.601681
 H     2.110639    -0.369838    -0.333140
 H     3.001199    -0.764177     1.884063
 H     2.645595    -0.976174     4.337683
```

```
 H     0.456148    -0.364837     5.355716
 H    -1.352616     0.603139     3.925281
 H    -0.935273     0.992899     1.494043
 H     0.971226     1.002741    -0.463055
   27
FN
 C     2.047283     0.267417     2.466910
 C     0.846509     0.455025     1.756791
 C    -0.364374     0.123190     2.420211
 C    -0.367954    -0.373138     3.735609
 C     0.834945    -0.542713     4.411283
 C     2.045103    -0.222764     3.771049
 S     0.794117     1.160083     0.119837
Cu     2.274760    -0.063547    -0.889807
 N    -1.555341     0.293278     1.682277
 C    -2.795599     0.291791     2.086965
 C    -3.942270     0.448747     1.234120
 C    -5.214161     0.492247     1.853608
 C    -6.364679     0.659713     1.086026
 C    -6.259108     0.783620    -0.305169
 C    -5.001950     0.738315    -0.933248
 C    -3.849543     0.570108    -0.175490
 H     2.989026     0.531867     1.980182
 H     2.992510    -0.355388     4.299243
 H     0.835819    -0.932515     5.431290
 H    -1.306368    -0.647766     4.222088
 H    -2.963785     0.173061     3.162028
 H    -5.287805     0.397686     2.940734
 H    -7.344016     0.694634     1.568484
 H    -7.160737     0.914190    -0.909088
 H    -4.930568     0.832395    -2.019169
 H    -2.881236     0.529879    -0.682957
 H    -1.349182     0.488429     0.687094
   27
FN'
   C  -0.107691  -0.001342  -3.327291
   C   0.062285   0.100938  -1.926390
   C  -1.106333  -0.094494  -1.137987
   C  -2.358284  -0.340531  -1.740935
   C  -2.485443  -0.422072  -3.119143
   C  -1.341536  -0.252892  -3.916104
   S   1.649487   0.466161  -1.226267
   C  -0.180800  -0.208622   1.155103
   N  -1.132813  -0.004924   0.276558
   C  -0.315171  -0.004716   2.573109
   C   0.764326  -0.422129   3.387475
   C   0.698811  -0.276148   4.771628
   C  -0.438830   0.293347   5.357392
   C  -1.513630   0.722574   4.559413
   C  -1.455262   0.579573   3.178121
   H  -3.236094  -0.477938  -1.101481
   H  -3.459562  -0.618167  -3.571456
   H  -1.415241  -0.320382  -5.004293
   H   0.775681   0.113641  -3.960915
   H  -2.292899   0.942372   2.574840
   H  -2.392154   1.176119   5.023906
   H  -0.490610   0.411365   6.442803
   H   1.533030  -0.603342   5.396193
   H   1.648626  -0.864601   2.920669
```

```
   H  -2.048022   0.252909   0.648117
   H   0.768790  -0.582479   0.768982
  Cu   2.577450   1.712402  -2.747167
   27
FCu
 C     2.367605   -1.692635    0.426073
 C     2.817594   -0.676272   -0.450148
 C     4.120192   -0.144115   -0.273971
 C     4.951303   -0.620426    0.736230
 C     4.492974   -1.632528    1.589444
 C     3.201748   -2.164466    1.432958
 C     2.052394   -0.123683   -1.541857
 N     0.889993   -0.492795   -2.003385
Cu    -0.237465   -2.147441   -1.653778
 S    -0.718724   -2.191621   -3.934389
 C    -0.456464   -0.493289   -4.049760
 C     0.279129    0.233865   -3.037486
 C     0.353445    1.631230   -3.116951
 C    -0.209703    2.305651   -4.203167
 C    -0.873503    1.600325   -5.231010
 C    -0.992748    0.223321   -5.158172
 H    -0.571300   -2.045567   -0.191145
 H     0.849217    2.191643   -2.321898
 H    -0.131154    3.394563   -4.255973
 H    -1.303898    2.143168   -6.075507
 H    -1.520638   -0.335057   -5.934793
 H     2.551859    0.701553   -2.073130
 H     4.473525    0.644752   -0.944530
 H     5.954095   -0.206169    0.862112
 H     5.141086   -2.008013    2.385790
 H     2.848337   -2.945950    2.109682
 H     1.358693   -2.094846    0.332603
   27
FNR
 C     1.905505    2.385105   -0.727114
 C     0.664497    1.806914   -0.457989
 C     0.180727    1.681700    0.858717
 C     0.958284    2.139095    1.926107
 C     2.201468    2.726290    1.662236
 C     2.675392    2.845589    0.349139
 S    -0.502712    1.195136   -1.678102
 C    -1.582360    0.456708   -0.184106
 N    -1.102701    1.112280    0.986265
 C    -1.347516   -1.037558   -0.253882
 C    -0.110836   -1.582430    0.196383
 C     0.213211   -2.918954   -0.112501
 C    -0.711251   -3.730445   -0.801573
 C    -1.956424   -3.212055   -1.161254
 C    -2.268155   -1.865980   -0.903082
 H     0.591562    2.031592    2.949524
 H     2.810227    3.088856    2.493778
 H     3.648860    3.302351    0.157398
 H     2.267090    2.488408   -1.752915
 H    -3.224971   -1.454087   -1.235765
 H    -2.687872   -3.848704   -1.664999
 H    -0.460628   -4.769721   -1.025943
 H     1.158393   -3.340532    0.239170
 H     0.543567   -0.984612    0.839368
 H    -2.633697    0.698219   -0.393136
```

```
 H    -1.784326     1.705954     1.452969
Cu     0.554666    -0.919120    -1.758696
   30
FS-H2O
 C     1.452357     0.838640    -2.950084
 C     0.769514     0.026245    -2.025686
 C    -0.153304    -0.932450    -2.499629
 C    -0.419538    -1.036645    -3.864999
 C     0.235841    -0.189463    -4.775397
 C     1.174442     0.740981    -4.316919
 C     1.053212     0.179383    -0.600262
 N     0.206386    -0.120938     0.330820
Cu    -1.828732    -0.028919    -0.002908
 S    -2.061061     0.621688     2.226610
 C    -0.367903     0.181244     2.689930
 C     0.593673    -0.100012     1.691004
 C     1.905205    -0.415418     2.097437
 C     2.253375    -0.421868     3.447389
 C     1.297701    -0.117224     4.424113
 C    -0.010131     0.192205     4.042239
 H    -0.758225     0.444479     4.797651
 H     1.567093    -0.122431     5.482690
 H     3.274633    -0.677817     3.739323
 H     2.646168    -0.694401     1.345226
 H    -2.686483    -0.440421     2.796190
 H     2.041239     0.591370    -0.336338
 H     2.192059     1.560487    -2.591832
 H     1.697907     1.386264    -5.026394
 H     0.029798    -0.275628    -5.845321
 H    -1.110473    -1.801672    -4.230632
 H    -0.630056    -1.613685    -1.790440
 O    -2.947840    -0.142200    -1.645856
 H    -3.813386     0.275083    -1.766468
 H    -2.493471    -0.133034    -2.506369
   30
FC-H2O
 C    -2.483526    -1.902104    -3.180626
 C    -2.094169    -1.691135    -1.816670
 C    -0.807889    -0.960089    -1.560410
 C    -0.165264    -0.289158    -2.676303
 C    -0.630348    -0.480211    -3.942562
 C    -1.788632    -1.305643    -4.199411
 S    -3.096159    -2.142726    -0.550372
Cu    -1.469034    -1.827564     1.119192
 N    -0.315660    -1.040872    -0.355430
 C     0.851637    -0.270735     0.078573
 C     0.762041    -0.126980     1.581729
 C     1.545635    -0.916912     2.435007
 C     1.369888    -0.846057     3.823953
 C     0.394932     0.005846     4.366758
 C    -0.395917     0.792162     3.518115
 C    -0.210250     0.728670     2.133065
 H    -3.377987    -2.496022    -3.380018
 H    -2.123052    -1.436310    -5.231886
 H    -0.113483    -0.020335    -4.788724
 H     0.731582     0.305028    -2.498223
 H     1.764243    -0.824985    -0.205441
 H     2.299696    -1.586779     2.012430
 H     2.001365    -1.447505     4.483336
```

```
 H     0.264748     0.067402     5.450421
 H    -1.147409     1.465827     3.937547
 H    -0.821183     1.349773     1.471175
 H     0.892845     0.720118    -0.406677
 O    -1.317966    -2.499857     2.983621
 H    -2.074393    -2.636142     3.572530
 H    -0.601964    -2.109505     3.519059
   30
FN-H2O
 C    -3.840050     0.480786    -0.180514
 C    -3.929838     0.458251     1.233721
 C    -5.196967     0.583307     1.850548
 C    -6.345726     0.731542     1.075931
 C    -6.243333     0.756980    -0.320611
 C    -4.990595     0.632010    -0.945653
 C    -2.783514     0.322835     2.093752
 N    -1.547415     0.243558     1.685632
 C    -0.358205     0.081062     2.423923
 C     0.856676     0.301444     1.717722
 C     2.056380     0.106962     2.433333
 C     2.047731    -0.274615     3.771766
 C     0.832769    -0.481238     4.451265
 C    -0.368273    -0.307385     3.775886
 S     0.806677     0.864491     0.037165
Cu     2.474872    -0.205218    -0.851358
 H     3.004055     0.281367     1.918240
 H     2.995274    -0.411765     4.298831
 H     0.830263    -0.786858     5.499490
 H    -1.312932    -0.495338     4.290761
 H    -2.949946     0.293368     3.175077
 H    -5.268817     0.565817     2.941762
 H    -7.321309     0.828226     1.557685
 H    -7.143303     0.872714    -0.929974
 H    -4.920095     0.650830    -2.035585
 H    -2.875186     0.379051    -0.685836
 H    -1.339994     0.350707     0.676416
 O     3.983260    -1.117895    -1.696343
 H     3.878948    -1.895371    -2.265700
 H     4.774115    -0.647295    -2.001724
   30
FNR-H2O
 C     0.121222     2.589155     0.036767
 C    -0.092344     1.211374     0.031482
 C     0.589925     0.357605     0.919209
 C     1.498994     0.894670     1.833046
 C     1.723315     2.276973     1.839479
 C     1.038259     3.119052     0.954409
 N     0.301237    -1.020132     0.783059
 C    -0.901769    -1.281858     0.075782
 S    -1.144875     0.300527    -1.105925
 C    -2.158610    -1.369702     0.912333
 C    -3.284850    -2.031354     0.387933
 C    -4.483209    -2.065963     1.106934
 C    -4.567094    -1.441515     2.361621
 C    -3.441998    -0.792234     2.892773
 C    -2.238590    -0.763432     2.177814
 H    -0.807746    -2.148653    -0.592381
 H     2.018975     0.235371     2.531869
 H     2.435609     2.701513     2.550797
```

```
 H     1.218346     4.196253     0.973520
 H    -0.405279     3.242520    -0.662821
 H     1.095546    -1.587960     0.496501
 H    -1.357893    -0.279433     2.602901
 H    -3.494971    -0.324888     3.879327
 H    -5.494049    -1.493030     2.939741
 H    -5.346539    -2.598550     0.699695
 H    -3.219906    -2.522319    -0.587692
Cu    -3.134735     0.882746    -0.268486
 O    -4.830047     1.252552     0.623876
 H    -5.651268     1.494216     0.169065
 H    -5.051984     0.576446     1.293507
   27
TS FS FN
 C     1.337705     0.461937     2.299765
 C     0.115379     0.008239     1.767692
 C    -0.876139    -0.423725     2.685990
 C    -0.659798    -0.434771     4.064505
 C     0.569926     0.009543     4.561170
 C     1.560387     0.459489     3.677737
 N    -0.229248    -0.018323     0.414605
 C     0.641100    -0.001356    -0.536880
 C     0.291611     0.002995    -1.948785
 C    -1.047728     0.082731    -2.390565
 C    -1.338150     0.072102    -3.750830
 C    -0.296746    -0.015739    -4.690559
 C     1.034800    -0.089910    -4.265466
 C     1.328600    -0.078504    -2.900740
 S    -2.442721    -0.994711     1.983288
 H    -1.435412    -0.791746     4.746618
 H     0.752054     0.004834     5.638201
 H     2.516347     0.816686     4.068140
 H     2.112417     0.834775     1.626238
 H    -1.859664    -0.928535     0.717393
 H     1.723205    -0.004471    -0.314087
 H     2.366795    -0.137802    -2.561167
 H     1.842024    -0.156422    -4.998637
 H    -0.528649    -0.022896    -5.758756
 H    -2.374469     0.134538    -4.091902
 H    -1.845850     0.159649    -1.648611
Cu    -3.257775     1.051394     1.605640
   27
TS FN FNR2
 C    -0.299246    -1.283454    -3.345889
 C    -0.028865    -0.774066    -2.060752
 C    -0.284217     0.588582    -1.752471
 C    -0.774718     1.438848    -2.744505
 C    -1.025724     0.932816    -4.029184
 C    -0.786792    -0.410746    -4.332917
 S     0.533520    -1.729518    -0.606611
 C     0.782700     0.097394     0.328251
 N    -0.061729     0.946118    -0.418148
 C     0.506964     0.007401     1.784968
 C     1.573616     0.053316     2.696786
 C     1.325198    -0.018748     4.070245
 C     0.011599    -0.144180     4.536607
 C    -1.056296    -0.201450     3.629825
 C    -0.810636    -0.130314     2.258318
 H    -0.959994     2.489979    -2.511575
```

```
 H    -1.410204     1.603184    -4.801346
 H    -0.994676    -0.794720    -5.333991
 H    -0.181220    -2.350154    -3.559251
 H    -1.642365    -0.200758     1.551023
 H    -2.080345    -0.309387     3.995176
 H    -0.182704    -0.201368     5.610643
 H     2.156846     0.026135     4.777435
 H     2.598382     0.158115     2.328785
 H    -0.837584     1.371118     0.084458
 H     1.848585     0.257267     0.112845
Cu     2.079905    -1.421411    -2.268725
   27
FNR2
   C  -0.265982  -0.999375  -2.810776
   C  -0.289925  -0.461385  -1.500909
   C  -1.330810   0.419591  -1.082601
   C  -2.296844   0.820278  -2.014969
   C  -2.244175   0.313092  -3.320199
   C  -1.246579  -0.584000  -3.724425
   S   0.746687  -0.938594  -0.067115
   C  -0.005162   0.528395   0.915842
   N  -1.273773   0.726598   0.250688
   C  -0.111665   0.232642   2.380406
   C   0.787760   0.831479   3.275027
   C   0.707291   0.550940   4.642372
   C  -0.272174  -0.328424   5.117063
   C  -1.172124  -0.928436   4.225326
   C  -1.091939  -0.652888   2.859340
   H  -3.095663   1.502934  -1.715864
   H  -3.006101   0.626177  -4.038116
   H  -1.239163  -0.980487  -4.741535
   H   0.467144  -1.763814  -3.086612
   H  -1.785740  -1.121288   2.156750
   H  -1.936179  -1.615154   4.597980
   H  -0.336661  -0.547105   6.185966
   H   1.406111   1.022428   5.337572
   H   1.548000   1.524278   2.901108
   H  -1.946015   1.352540   0.681640
   H   0.690295   1.376143   0.748428
  Cu   1.496028   0.488179  -1.920188
   27
TS FNR2 FNR3
 C    -0.247436    -1.326308    -3.329890
 C     0.013657    -0.789853    -2.037678
 C    -0.311810     0.572012    -1.733641
 C    -0.816221     1.398439    -2.748121
 C    -1.041857     0.862785    -4.022314
 C    -0.764668    -0.478681    -4.320834
 S     0.460805    -1.684064    -0.520726
 C     0.747328    -0.003999     0.328378
 N    -0.130921     0.876471    -0.414724
 C     0.476882    -0.049414     1.802086
 C     1.550068    -0.034449     2.704885
 C     1.308997    -0.091600     4.081122
 C    -0.005153    -0.162787     4.556144
 C    -1.079601    -0.178361     3.655800
 C    -0.841616    -0.125750     2.281393
 H    -1.059663     2.441533    -2.532560
 H    -1.446645     1.512312    -4.802217
```

```
 H    -0.966374    -0.874906    -5.317837
 H    -0.109203    -2.394494    -3.523022
 H    -1.672915    -0.145389     1.572352
 H    -2.105268    -0.234712     4.028584
 H    -0.194813    -0.205454     5.631722
 H     2.146814    -0.076513     4.782354
 H     2.576092     0.027828     2.329652
 H    -0.277373     1.816587    -0.061287
 H     1.815896     0.242490     0.145340
Cu     1.974996    -0.893723    -2.534960
   27
FNR3
   C  -0.452879  -0.972719  -2.908072
   C  -0.175435  -0.440403  -1.606722
   C  -0.505540   0.936429  -1.317800
   C  -1.031879   1.755843  -2.335979
   C  -1.307970   1.202405  -3.591303
   C  -1.027689  -0.141858  -3.885609
   S   0.132771  -1.334191  -0.093402
   C   0.494913   0.311745   0.745294
   N  -0.328191   1.244526  -0.008351
   C   0.216876   0.298015   2.219607
   C   1.284958   0.296081   3.128017
   C   1.034854   0.268448   4.503833
   C  -0.283019   0.245204   4.972745
   C  -1.352590   0.246819   4.066557
   C  -1.105574   0.268757   2.692836
   H  -1.275398   2.799249  -2.122319
   H  -1.747643   1.839048  -4.362831
   H  -1.251799  -0.548768  -4.873427
   H  -0.293249  -2.037025  -3.101429
   H  -1.933565   0.259003   1.979532
   H  -2.381497   0.226582   4.434147
   H  -0.479438   0.225714   6.047783
   H   1.869299   0.268388   5.209276
   H   2.314177   0.319169   2.757456
   H  -0.452831   2.187121   0.347124
   H   1.573473   0.513495   0.559784
  Cu   1.606503  -0.012229  -2.537403
   27
TS FNR3 G
 C     0.205924    -1.363342    -3.380437
 C     0.007651    -0.914736    -2.065089
 C    -0.400557     0.424279    -1.814208
 C    -0.586109     1.330165    -2.870270
 C    -0.388600     0.869605    -4.171931
 C     0.002104    -0.460051    -4.424999
 S     0.056827    -1.837055    -0.562814
 C     0.064396    -0.284390     0.321732
 N    -0.563018     0.652555    -0.463488
 C    -0.007872    -0.213540     1.788861
 C    -0.018899     1.046504     2.421212
 C    -0.095816     1.135171     3.809541
 C    -0.150060    -0.031756     4.584428
 C    -0.122228    -1.286711     3.965179
 C    -0.046480    -1.380620     2.574890
 H    -0.891678     2.360606    -2.673552
 H    -0.532165     1.556359    -5.009264
 H     0.153807    -0.790000    -5.455214
```

```
 H     0.500905    -2.396055    -3.580095
 H    -0.032626    -2.367345     2.104713
 H    -0.161959    -2.197542     4.566841
 H    -0.206854     0.039189     5.673419
 H    -0.102487     2.115469     4.291806
 H     0.064306     1.965851     1.833600
 H    -0.771817     1.575423    -0.093547
 H     1.628447     0.140609     0.009806
Cu     2.394856     0.311357    -1.381121
   27
G
 C    -0.939267    -0.789751    -2.750123
 C    -0.772892    -0.315544    -1.429036
 C    -0.379820     1.009951    -1.182702
 C    -0.149662     1.920234    -2.229576
 C    -0.330295     1.467400    -3.530492
 C    -0.729401     0.128998    -3.800290
 S    -0.945180    -1.194025     0.076728
 C    -0.506218     0.209264     0.990421
 N    -0.247814     1.244009     0.179221
 C    -0.411692     0.257439     2.435388
 C     0.327158     1.285381     3.067555
 C     0.413484     1.330145     4.456030
 C    -0.229578     0.354026     5.231136
 C    -0.958472    -0.672331     4.614452
 C    -1.050495    -0.725373     3.226218
 H     0.163804     2.946359    -2.025495
 H    -0.165322     2.150234    -4.366432
 H    -0.941999    -0.171318    -4.829635
 H    -1.320122    -1.795222    -2.944366
 H    -1.638644    -1.517766     2.755415
 H    -1.460637    -1.429965     5.220070
 H    -0.157969     0.391689     6.321011
 H     0.993955     2.119846     4.938192
 H     0.869396     2.030944     2.479598
 H    -0.001307     2.159182     0.551462
 H     2.596974    -1.405285    -3.191161
Cu     1.190607    -0.878144    -3.357042
   25
2-H+
 C     0.147235     1.065749     2.376972
 C     0.080916    -0.195155     1.740357
 C     0.009776    -1.366861     2.527156
 C    -0.004096    -1.274866     3.916917
 C     0.054830    -0.020170     4.538362
 C     0.132082     1.148181     3.766797
 C     0.087507    -0.283328     0.291536
 N    -0.223729     0.728247    -0.526038
 C    -0.156540     0.465910    -1.891449
 C     0.238332    -0.865044    -2.131036
 S     0.518797    -1.696635    -0.607303
 C    -0.437753     1.345401    -2.943907
 C    -0.309113     0.854227    -4.241189
 C     0.087962    -0.477144    -4.484121
 C     0.366123    -1.354682    -3.435901
 H    -0.746338     2.375876    -2.752801
 H    -0.520367     1.513634    -5.085923
 H     0.179949    -0.830075    -5.513752
 H     0.672775    -2.384807    -3.628951
```

```
 H    -0.059904    -2.348099     2.050127
 H    -0.067699    -2.183749     4.519273
 H     0.043947     0.048686     5.628997
 H     0.193050     2.124442     4.253089
 H     0.248675     1.984923     1.792911
 H    -0.536419     1.625336    -0.160126
2
CuH
Cu    0.0000000    0.0000000   -0.7358005
H     0.0000000    0.0000000    0.7358005
   26
Cu(1-half)+
 C     2.205058     0.311023     2.115043
 C     0.899393     0.413189     1.596537
 C    -0.166688     0.721505     2.476043
 C     0.063522     0.882957     3.838052
 C     1.367961     0.748981     4.345017
 C     2.435352     0.471273     3.483934
 C     0.686421     0.157745     0.180090
 N    -0.487854    -0.084903    -0.306534
Cu    -2.066299    -0.680132     0.861046
 S    -3.034140    -1.722284    -0.884573
 C    -1.907703    -1.071417    -2.033654
 C    -0.745290    -0.287951    -1.666273
 C     0.053949     0.257667    -2.679760
 C    -0.232334     0.012381    -4.025781
 C    -1.336246    -0.782209    -4.393207
 C    -2.157248    -1.318391    -3.413170
 H    -3.019506    -1.931142    -3.686400
 H    -1.549393    -0.970070    -5.447876
 H     0.409080     0.444489    -4.798058
 H     0.900737     0.894257    -2.415217
 H     1.579371     0.126869    -0.464868
 H     3.035945     0.087527     1.439962
 H     3.449085     0.379058     3.880392
 H     1.549089     0.877009     5.415228
 H    -0.760774     1.135018     4.509527
 H    -1.171487     0.927553     2.074500
2
ZnCl+
Zn    0.0000000    0.0000000   -1.0425154
Cl    0.0000000    0.0000000    1.0425154
   52
ZnCl-A
 C     0.155306    -2.376397    -2.563131
 C    -0.108545    -1.988952    -1.235324
 C     0.900392    -2.112228    -0.257938
 C     2.169991    -2.564162    -0.616505
 C     2.439631    -2.900811    -1.949761
 C     1.430945    -2.813472    -2.920494
 C    -1.438941    -1.510573    -0.865895
 N    -1.635092    -0.590914     0.017423
 C    -2.928863    -0.410203     0.576468
 C    -3.559524     0.855485     0.616034
 S    -3.110436     2.274923    -0.362324
 C    -3.522395    -1.495448     1.235397
 C    -4.740008    -1.348600     1.904887
 C    -5.360697    -0.098434     1.953442
 C    -4.764940     0.999077     1.325202
```

```
Zn    -0.186034     0.522962     1.032014
 N     1.388379     0.905359    -0.264887
 C     2.682663     0.833061    -0.160795
 C     3.497061     0.323363     0.920869
 C     4.895589     0.328908     0.697435
 C     5.771928    -0.172062     1.657537
 C     5.264323    -0.681361     2.859924
 C     3.881066    -0.684961     3.097267
 C     3.000242    -0.189359     2.139840
 S    -1.038845     2.676906    -0.014794
 C    -0.299867     2.116221    -1.561961
 C     0.849726     1.299895    -1.520992
 C     1.403809     0.847286    -2.731274
 C     0.855838     1.237284    -3.952132
 C    -0.261036     2.081536    -3.984654
 C    -0.835909     2.520183    -2.790741
 H    -2.310341    -1.981416    -1.350338
 H     2.242118     0.148714    -2.702573
 H     1.296050     0.871017    -4.882632
 H    -0.690217     2.395077    -4.939131
 H    -1.713447     3.169884    -2.811380
 H     3.265848     1.187268    -1.024637
 H     5.288097     0.728677    -0.242189
 H     6.848801    -0.163536     1.473888
 H     5.948255    -1.072416     3.617874
 H     3.484699    -1.071419     4.039175
 H     1.935791    -0.190117     2.368658
 H    -2.992858    -2.450781     1.249569
 H    -5.186456    -2.208308     2.410013
 H    -6.300449     0.033356     2.494385
 H    -5.243630     1.980419     1.369363
 H     0.670091    -1.906623     0.792261
 H     2.944111    -2.668034     0.147261
 H     3.433198    -3.260804    -2.229775
 H     1.640020    -3.099566    -3.954245
 H    -0.636109    -2.311106    -3.314624
Cl    -0.372713    -0.032766     3.128817
   52
ZnCl-B
 C     0.258606    -2.252186    -1.521250
 C     1.345174    -2.179890    -0.630315
 C     2.628364    -2.556938    -1.077075
 C     2.829356    -2.932922    -2.405442
 C     1.744333    -2.971658    -3.291984
 C     0.456384    -2.644357    -2.843598
 C     1.197078    -1.767008     0.759289
 N     0.279275    -0.993247     1.236285
Zn    -1.216102     0.207516     0.295845
 N    -0.258160     0.798278    -1.595484
 C     1.028557     0.843660    -1.781743
 C     2.030972     1.078409    -0.765202
 C     3.362631     0.705171    -1.059515
 C     4.372943     0.906388    -0.122243
 C     4.069606     1.512948     1.106214
 C     2.756672     1.915423     1.393270
 C     1.737485     1.700548     0.468415
 C     0.272569    -0.726358     2.632324
 C    -0.986269    -0.681535     3.312377
 C    -0.991970    -0.435380     4.708425
```

```
 C     0.192847    -0.210496     5.402125
 C     1.416586    -0.232807     4.716343
 C     1.454448    -0.489663     3.340386
 S    -2.477109    -0.908926     2.469441
 S    -2.969021    -0.593712    -1.187424
 C    -2.402874     0.163888    -2.617818
 C    -1.111507     0.809015    -2.700589
 C    -0.775318     1.481999    -3.888136
 C    -1.636279     1.479015    -4.986493
 C    -2.878490     0.813094    -4.928604
 C    -3.254829     0.171722    -3.762181
 H     1.952566    -2.173211     1.450896
 H     0.158294     2.044844    -3.939843
 H    -1.345953     2.011963    -5.895547
 H    -3.546619     0.820617    -5.792586
 H    -4.221855    -0.331204    -3.689589
 H     1.420856     0.675564    -2.798056
 H     3.588811     0.241234    -2.023034
 H     5.399777     0.609729    -0.349264
 H     4.865778     1.690641     1.834566
 H     2.525749     2.408582     2.340138
 H     0.724229     2.041672     0.691368
 H     2.406749    -0.476693     2.808019
 H     2.349166    -0.042441     5.253499
 H     0.168156    -0.009769     6.475582
 H    -1.953940    -0.414442     5.225058
 H     3.470306    -2.532035    -0.380030
 H     3.828290    -3.211351    -2.749615
 H     1.898377    -3.282681    -4.328597
 H    -0.395909    -2.712329    -3.524246
 H    -0.745755    -2.031706    -1.161609
Cl    -1.670614     2.104563     1.371249
   52
ZnCl-C
 C     1.087954    -1.614729    -0.418460
 C     1.416332    -1.121004     0.857462
 C     2.769462    -0.918428     1.193206
 C     3.770468    -1.153198     0.251151
 C     3.432181    -1.620753    -1.025138
 C     2.090524    -1.858658    -1.355591
 C     0.403137    -0.906518     1.881640
 N    -0.826798    -0.524894     1.676908
Zn    -1.634109     0.284140    -0.042350
 N    -0.454583     0.695089    -1.763815
 C     0.750907     1.183297    -1.768388
 C     1.412392     1.819658    -0.650443
 C     2.822280     1.898154    -0.690640
 C     3.527291     2.469721     0.366209
 C     2.830770     2.990091     1.464314
 C     1.427436     2.953372     1.496393
 C     0.716168     2.378100     0.447083
 C    -1.740438    -0.709224     2.743166
 C    -1.779533    -1.973131     3.450973
 C    -2.761859    -2.125144     4.473112
 C    -3.653916    -1.107736     4.780139
 C    -3.591684     0.110737     4.081535
 C    -2.646235     0.304083     3.069927
 S    -0.750021    -3.296769     3.069450
 S    -2.603580    -1.478674    -1.416512
```

```
 C    -2.030433    -0.811829    -2.894451
 C    -1.036242     0.237153    -2.952590
 C    -0.712213     0.787411    -4.202246
 C    -1.286357     0.293109    -5.375508
 C    -2.216904    -0.765036    -5.333286
 C    -2.582719    -1.305462    -4.112783
 H     0.746377    -1.019421     2.919149
 H    -0.026698     1.634981    -4.256153
 H    -1.016430     0.743369    -6.334167
 H    -2.661582    -1.142916    -6.256554
 H    -3.319492    -2.110116    -4.057994
 H     1.357085     1.084406    -2.681882
 H     3.357763     1.485905    -1.549257
 H     4.618180     2.517305     0.334777
 H     3.381183     3.449867     2.289597
 H     0.887533     3.400873     2.334461
 H    -0.375186     2.429905     0.445906
 H    -2.616704     1.245330     2.520201
 H    -4.282812     0.920752     4.327512
 H    -4.397107    -1.252707     5.567741
 H    -2.792753    -3.074049     5.012581
 H     3.029294    -0.565626     2.194772
 H     4.817401    -0.983961     0.513711
 H     4.218273    -1.826090    -1.756778
 H     1.831446    -2.260580    -2.338453
 H     0.047586    -1.842177    -0.653568
Cl    -2.953036     2.052022     0.123928
   52
ZnCl-D
 C    -1.374363    -2.284612    -1.247364
 C    -0.154458    -1.604345    -1.087387
 C     0.509546    -1.112317    -2.214532
 C    -0.038595    -1.285268    -3.492272
 C    -1.250808    -1.965674    -3.648472
 C    -1.917508    -2.467868    -2.525100
 C     0.431613    -1.401006     0.290820
 N    -0.477542    -0.782841     1.231642
 C    -0.547716    -1.404709     2.415394
 C     0.203967    -2.634407     2.528213
 S     1.032125    -3.009125     1.049570
 C    -1.305044    -0.943593     3.533588
 C    -1.303008    -1.693343     4.692622
 C    -0.565144    -2.904804     4.786395
 C     0.188819    -3.378556     3.711750
Zn    -1.499576     0.903851     0.694457
 N    -0.144356     1.739061    -0.720822
 C     1.139127     1.812497    -0.528026
 C     1.821024     1.720071     0.747658
 C     3.190482     1.362914     0.718656
 C     3.898157     1.178529     1.904560
 C     3.254402     1.376320     3.134392
 C     1.908270     1.769943     3.173984
 C     1.191011     1.945631     1.992866
 S    -2.899002     0.433258    -1.213325
 C    -1.925469     1.283749    -2.351548
 C    -0.672441     1.910590    -2.012810
 C    -0.032927     2.698478    -2.982762
 C    -0.551002     2.814576    -4.274676
 C    -1.738084     2.150827    -4.632535
```

```
 C    -2.415140     1.402357    -3.682125
 H     1.336038    -0.771733     0.210077
 H     0.867251     3.256472    -2.718728
 H    -0.031715     3.439374    -5.005698
 H    -2.138339     2.244752    -5.644498
 H    -3.354878     0.905346    -3.932925
 H     1.802606     1.895165    -1.403505
 H     3.689421     1.219153    -0.244547
 H     4.951640     0.891126     1.875109
 H     3.809928     1.241698     4.066242
 H     1.417283     1.954348     4.132368
 H     0.159200     2.297779     2.047887
 H    -1.856653    -0.004461     3.449803
 H    -1.876454    -1.349478     5.556671
 H    -0.587195    -3.475531     5.717934
 H     0.753305    -4.309757     3.792889
 H     1.459585    -0.584779    -2.094492
 H     0.484282    -0.888919    -4.366064
 H    -1.674772    -2.106632    -4.645609
 H    -2.863810    -3.001720    -2.639598
 H    -1.889770    -2.679300    -0.367948
Cl    -2.413310     2.196910     2.221819
   52
ZnCl-D'
 C    -1.868782    -0.701332    -2.382847
 C    -0.791983    -1.402416    -1.813299
 C     0.266436    -1.820314    -2.624170
 C     0.249194    -1.549716    -3.998863
 C    -0.827585    -0.860015    -4.565796
 C    -1.885946    -0.432133    -3.756262
 C    -0.781459    -1.701397    -0.331865
 N    -1.087633    -0.548510     0.485148
 C    -2.075230    -0.739497     1.369197
 C    -2.714319    -2.035967     1.327902
 S    -2.009332    -3.053904     0.111826
 C    -2.522091     0.232367     2.313586
 C    -3.567613    -0.091803     3.154464
 C    -4.195656    -1.365942     3.094503
 C    -3.773400    -2.340096     2.188798
Zn     0.015331     1.150972     0.228505
 N     1.934427     0.524266    -0.468294
 C     2.959571     0.478882     0.337585
 C     2.925192     0.206519     1.755190
 C     4.083377     0.524467     2.502190
 C     4.116524     0.315463     3.878915
 C     3.001881    -0.237196     4.523112
 C     1.856798    -0.584789     3.789489
 C     1.813906    -0.363516     2.418076
 S    -0.273656     2.030032    -2.004100
 C     1.178649     1.367227    -2.650613
 C     2.147788     0.664313    -1.849724
 C     3.274185     0.117043    -2.484609
 C     3.490138     0.297047    -3.852642
 C     2.569862     1.016760    -4.634106
 C     1.427648     1.533209    -4.041733
 H     0.214574    -2.092026    -0.050489
 H     3.984080    -0.473280    -1.902213
 H     4.381659    -0.134092    -4.315243
 H     2.744956     1.156741    -5.703095
```

```
 H     0.692939     2.081023    -4.635500
 H     3.959871     0.689713    -0.072779
 H     4.950792     0.952886     1.991667
 H     5.008593     0.578103     4.451929
 H     3.026985    -0.407307     5.602579
 H     0.996381    -1.027764     4.296154
 H     0.928255    -0.656156     1.855974
 H    -2.013733     1.198001     2.360998
 H    -3.919171     0.642778     3.882866
 H    -5.023102    -1.588238     3.772553
 H    -4.259439    -3.317268     2.152557
 H     1.110839    -2.356007    -2.182228
 H     1.083715    -1.872777    -4.625270
 H    -0.840768    -0.653130    -5.638696
 H    -2.727881     0.110943    -4.192096
 H    -2.697124    -0.376767    -1.747822
Cl     0.150859     2.553960     1.904157
   52
ZnCl-D''
 C    -2.062843    -1.124337    -0.424614
 C    -1.046645    -2.080715    -0.279193
 C    -0.795934    -2.988489    -1.314924
 C    -1.554908    -2.945115    -2.488865
 C    -2.563062    -1.986977    -2.632467
 C    -2.815500    -1.074532    -1.598737
 C    -0.238757    -2.149017     0.999513
 N     0.256652    -0.862583     1.435693
 C    -0.077972    -0.531960     2.688190
 C    -0.895287    -1.493610     3.394334
 S    -1.239765    -2.877760     2.410080
 C     0.307356     0.676552     3.342977
 C    -0.121352     0.894414     4.636746
 C    -0.929494    -0.057279     5.317988
 C    -1.315628    -1.249601     4.706500
Zn     1.394226     0.218196     0.137326
 N     0.373755     0.652057    -1.688156
 C    -0.101659     1.845689    -1.912214
 C    -0.580303     2.761066    -0.905019
 C    -0.711597     4.122887    -1.260192
 C    -1.141556     5.057633    -0.320899
 C    -1.471529     4.639056     0.975337
 C    -1.376949     3.284026     1.331363
 C    -0.933186     2.351714     0.401745
 S     2.546836    -1.469926    -1.170287
 C     1.650010    -1.229717    -2.614587
 C     0.629745    -0.214456    -2.752857
 C    -0.103458    -0.160534    -3.949845
 C     0.184701    -1.018540    -5.010070
 C     1.206011    -1.984621    -4.898657
 C     1.923174    -2.087318    -3.720579
 H     0.619914    -2.830898     0.844318
 H    -0.931229     0.543780    -4.040892
 H    -0.398080    -0.946117    -5.931965
 H     1.424627    -2.652524    -5.734997
 H     2.712046    -2.834994    -3.612163
 H    -0.132807     2.219534    -2.947993
 H    -0.453927     4.440991    -2.274299
 H    -1.224033     6.111787    -0.594733
 H    -1.814731     5.371235     1.710917
```

```
 H    -1.649953     2.959669     2.337991
 H    -0.892994     1.296781     0.669155
 H     0.945460     1.386534     2.812097
 H     0.173579     1.810691     5.153959
 H    -1.248598     0.146732     6.342977
 H    -1.930848    -1.977389     5.239826
 H    -0.000156    -3.729942    -1.202479
 H    -1.354718    -3.658066    -3.292061
 H    -3.159090    -1.953905    -3.548069
 H    -3.609665    -0.331085    -1.704957
 H    -2.270559    -0.426054     0.389888
Cl     2.443068     2.019591     0.806789
   52
ZnCl-TS AD
 C     0.299558    -4.801076    -3.193224
 C     1.122870    -4.697273    -2.061591
 C     2.488947    -4.426147    -2.228751
 C     3.020973    -4.246400    -3.508547
 C     2.193945    -4.341279    -4.631964
 C     0.831645    -4.619802    -4.471129
 C     0.621029    -4.982898    -0.674044
 N     1.234667    -4.301426     0.399021
 C     0.459442    -4.411484     1.513667
 C    -0.944511    -4.678191     1.278615
 S    -1.284493    -4.699269    -0.403131
 C     0.891284    -4.170420     2.838501
 C    -0.035573    -4.231526     3.863596
 C    -1.411597    -4.504480     3.621013
 C    -1.880046    -4.711387     2.334884
Zn     1.271190    -2.206756     0.114578
 N     1.767742    -1.465001    -1.765355
 C     2.830325    -0.732160    -1.946398
 C     4.040541    -0.761860    -1.158415
 C     4.933811     0.325393    -1.307484
 C     6.116746     0.376256    -0.574475
 C     6.435984    -0.671885     0.299458
 C     5.573781    -1.770331     0.436326
 C     4.384738    -1.818121    -0.283043
 S    -1.059620    -2.084187    -0.699022
 C    -0.601118    -1.759967    -2.353450
 C     0.749499    -1.481603    -2.735359
 C     1.028150    -1.271121    -4.097224
 C     0.010785    -1.271906    -5.049566
 C    -1.319055    -1.510153    -4.671068
 C    -1.616529    -1.757748    -3.336391
 H     0.608259    -6.077804    -0.478519
 H     2.061551    -1.137025    -4.418415
 H     0.258946    -1.098246    -6.099610
 H    -2.115385    -1.509479    -5.418759
 H    -2.645650    -1.954105    -3.026828
 H     2.826968    -0.003990    -2.772239
 H     4.679376     1.136680    -1.995427
 H     6.793473     1.226600    -0.683899
 H     7.367053    -0.638654     0.871236
 H     5.834572    -2.589942     1.109409
 H     3.741357    -2.691763    -0.181209
 H     1.937614    -3.924557     3.017176
 H     0.294250    -4.062279     4.891632
 H    -2.105864    -4.545016     4.463329
```

```
 H    -2.937099    -4.903770     2.140325
 H     3.134982    -4.374468    -1.351999
 H     4.088357    -4.041704    -3.625686
 H     2.610112    -4.205805    -5.633525
 H     0.178631    -4.694723    -5.343523
 H    -0.766055    -5.020695    -3.087815
Cl     1.953673    -1.122269     1.876378
   52
ZnCl-TS D ES
 C    -0.415036    -3.017284    -1.219856
 C     0.150957    -4.084989    -1.930693
 C    -0.223093    -4.318630    -3.261920
 C    -1.163218    -3.491877    -3.878487
 C    -1.725527    -2.423150    -3.170022
 C    -1.351335    -2.187549    -1.841512
 C     1.161582    -4.991625    -1.274393
 N     1.940989    -4.459110    -0.240615
 C     2.142568    -5.294021     0.782004
 C     1.456570    -6.566443     0.677353
 S     0.518659    -6.632654    -0.767399
 C     2.994767    -5.036589     1.896744
 C     3.119535    -6.012742     2.861435
 C     2.434621    -7.258099     2.749970
 C     1.617062    -7.550676     1.662857
Zn     3.341917    -3.054408    -0.984648
 N     2.359213    -1.586940    -2.110625
 C     2.344374    -0.346956    -1.715730
 C     2.404768     0.090336    -0.337591
 C     2.809740     1.418705    -0.080381
 C     2.907180     1.884391     1.229251
 C     2.570749     1.038929     2.294816
 C     2.132189    -0.270799     2.050298
 C     2.050625    -0.744789     0.745370
 S     3.520980    -4.293009    -3.081119
 C     2.612008    -3.122686    -4.014641
 C     2.094461    -1.910239    -3.458299
 C     1.283568    -1.093754    -4.264328
 C     1.039385    -1.411544    -5.600379
 C     1.590689    -2.571927    -6.163827
 C     2.363035    -3.416778    -5.375340
 H     1.975761    -5.158723    -2.144832
 H     0.808888    -0.212007    -3.831601
 H     0.406883    -0.754567    -6.202391
 H     1.406771    -2.818759    -7.211985
 H     2.787383    -4.330937    -5.796715
 H     2.292029     0.453029    -2.470419
 H     3.066181     2.074622    -0.917344
 H     3.239800     2.906642     1.423536
 H     2.638448     1.406259     3.322108
 H     1.851070    -0.917464     2.884691
 H     1.675561    -1.751638     0.555519
 H     3.543415    -4.093050     1.934657
 H     3.766679    -5.839921     3.724509
 H     2.562797    -8.006258     3.536281
 H     1.110043    -8.514410     1.584056
 H     0.236149    -5.139092    -3.819458
 H    -1.447258    -3.673596    -4.917369
 H    -2.459828    -1.774187    -3.653966
 H    -1.797677    -1.360391    -1.283683
```

```
 H    -0.124449    -2.842435    -0.181967
Cl     4.912429    -2.450147     0.400700
   52
ZnCl-ES
 C    -1.662544    -1.748499    -1.241290
 C    -1.314103    -2.515945    -0.115204
 C    -1.119158    -3.904422    -0.249944
 C    -1.243993    -4.506363    -1.504806
 C    -1.579031    -3.733890    -2.625234
 C    -1.793932    -2.357746    -2.489750
 C    -1.148611    -1.860142     1.188128
 N    -0.478104    -0.739344     1.384417
 C    -0.518417    -0.326137     2.720711
 C    -1.252903    -1.197116     3.560251
 S    -1.886268    -2.525342     2.615845
 C     0.088075     0.821777     3.259568
 C    -0.063815     1.068475     4.620847
 C    -0.801492     0.197422     5.448710
 C    -1.403266    -0.947526     4.930122
Zn     0.796154     0.144523     0.024980
 N     0.079967     0.984286    -1.780298
 C    -0.072347     2.274027    -1.834146
 C    -0.401478     3.111672    -0.698795
 C    -0.044883     4.475071    -0.750165
 C    -0.290829     5.306289     0.342137
 C    -0.924000     4.791895     1.480683
 C    -1.319298     3.446190     1.526211
 C    -1.059449     2.610216     0.445045
 S     1.840298    -1.544259    -1.496796
 C     1.029670    -0.932052    -2.988423
 C     0.251118     0.247048    -2.975297
 C    -0.401278     0.625706    -4.165125
 C    -0.249754    -0.115555    -5.336533
 C     0.556928    -1.259081    -5.345423
 C     1.197210    -1.660295    -4.171091
 H     1.015179    -2.607143    -1.300963
 H    -1.059932     1.496657    -4.157406
 H    -0.769968     0.198795    -6.244522
 H     0.685160    -1.840376    -6.261286
 H     1.827774    -2.552391    -4.167400
 H     0.077761     2.791080    -2.794848
 H     0.449576     4.870104    -1.642031
 H     0.007050     6.356746     0.307559
 H    -1.124930     5.446471     2.332674
 H    -1.832184     3.053547     2.406699
 H    -1.398852     1.572290     0.470889
 H     0.681444     1.479970     2.624152
 H     0.406684     1.952984     5.056551
 H    -0.899430     0.418025     6.514293
 H    -1.970967    -1.626107     5.570152
 H    -0.846870    -4.502486     0.623431
 H    -1.078608    -5.581554    -1.608949
 H    -1.676654    -4.208030    -3.605016
 H    -2.050426    -1.753441    -3.362388
 H    -1.831118    -0.676444    -1.131922
Cl     2.351609     1.516702     0.733280
   28
ZnCl-FS
 C     1.297970    -0.663377    -2.696262
```

```
 C     0.333977    -0.017254    -1.882961
 C    -0.739477     0.671574    -2.496955
 C    -0.863015     0.671436    -3.882559
 C     0.079702    -0.002931    -4.675231
 C     1.163024    -0.666027    -4.082120
 C     0.529550    -0.097816    -0.456036
 N    -0.359602     0.109136     0.480225
Zn    -2.368857     0.145047     0.231379
 S    -2.486689    -0.930936     2.447809
 C    -0.822577    -0.352801     2.851074
 C     0.050417     0.122124     1.843131
 C     1.299357     0.636847     2.230340
 C     1.678759     0.648883     3.574303
 C     0.812554     0.165003     4.559787
 C    -0.444528    -0.328733     4.196936
 H    -1.133965    -0.697264     4.960027
 H     1.104590     0.183960     5.612053
 H     2.652407     1.058967     3.852924
 H     1.963363     1.062903     1.475104
 H    -2.180382    -2.165920     1.963578
 H     1.539024    -0.393987    -0.133159
 H     2.143832    -1.174009    -2.226920
 H     1.902404    -1.176683    -4.703184
 H    -0.023334     0.003610    -5.763519
 H    -1.691330     1.209131    -4.349411
 H    -1.458410     1.245300    -1.911731
Cl    -3.978765     0.733814    -1.018622
   27
Zn(half-1)Cl+
 C    -1.977895    -1.296828    -3.646893
 C    -1.855483    -1.121774    -2.235040
 C    -0.758401    -0.329174    -1.715076
 C     0.102782     0.299456    -2.624713
 C    -0.053543     0.118020    -4.002481
 C    -1.090918    -0.690318    -4.516215
 S    -3.029631    -1.860359    -1.223570
 N    -0.610237    -0.186847    -0.325611
 C     0.588782    -0.010970     0.181997
 C     0.913169     0.333177     1.537162
 C     2.250098     0.107010     1.959603
 C     2.630725     0.391859     3.266247
 C     1.691564     0.928937     4.160759
 C     0.374858     1.190239     3.746302
 C    -0.016062     0.900813     2.444341
Zn    -2.280804    -0.773283     0.746827
 H    -2.798074    -1.911840    -4.024895
 H    -1.200743    -0.822359    -5.594755
 H     0.633507     0.621088    -4.687833
 H     0.888613     0.962857    -2.258440
 H     1.450822    -0.165800    -0.485385
 H     2.974575    -0.308937     1.253726
 H     3.655678     0.203530     3.593117
 H     1.991289     1.159405     5.186543
 H    -0.344799     1.626704     4.442211
 H    -1.030094     1.143067     2.129644
Cl    -3.099779    -0.507675     2.692429
```