Electronic Supporting Information for:

Cycloaddition of Alkynes to Diimino Mo$_3$S$_4$ Cubane-Type Clusters: A combined experimental and theoretical approach

Jose A. Pino-Chamorro,$^a$ Yuliya A. Laricheva,$^b$ Eva Guillamón,$^c$ María Jesús Fernández-Trujillo,$^a$ Emilio Bustelo,$^a$ Artem L. Gushchin,$^b*$ Nikita Y. Shmelev,$^b$ Pavel A. Abramov,$^b$ Maxim N. Sokolov,$^b*$ Rosa Llusar,$^c*$ Manuel G. Basallote,$^a*$ and Andrés G. Algarra$^{*a}$

$^a$Departamento de Ciencia de los Materiales e Ingeniería Metalúrgica y Química Inorgánica, Facultad de Ciencias, Instituto de Biomoléculas, Universidad de Cádiz, 11510 Puerto Real, Cádiz, Spain. E-mail: manuel.basallote@uca.es; andres.algarra@uca.es

$^b$Nikolaev Institute of Inorganic Chemistry, Siberian Branch of the Russian Academy of Sciences and Novosibirsk State University, 630090 Novosibirsk, Russia. E-mail: gushchin@niic.nsc.ru

$^c$Department de Química Física i Analítica, Universitat Jaume I, Av. Sos Baynat s/n, 12071 Castelló, Spain. E-mail: rosa.llusar@uji.es
Figure S1. UV-Vis spectrum of cluster [1]PF₆ in acetonitrile solution at 25.0 °C.
Figure S2. ESI-MS spectra of a solution 10^{-3} M of: a) [Mo_3S_4Cl_3(dbppy)_3]^+ ([1]^+); b) [W_3S_4Cl_3(dbppy)_3]^+ ([2]^+). In both cases the cluster concentration was 10^{-3} M in acetonitrile, and the measurements were performed at 20 V.
**Figure S3.** Plot of the dependence of [Alkyne] on the rate constants for the reaction of [1]PF$_6$ with an excess of dmad (circles) in acetonitrile solution, and also in the presence of 0.01 M Bu$_4$NPF$_6$ (triangles), or 0.01 M trifluoroacetic acid (squares).

**Figure S4.** DFT-optimised structures of the transition state and type I product of the [3+2] cycloaddition reaction between [1]$^+$ and acetylene. Selected distances are given in Å.
Table S1. Crystallographic data for [1]Cl·5H₂O.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>[1]Cl·5H₂O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical formula</td>
<td>C₄₄H₈₂Cl₄Mo₃N₆O₅S₄</td>
</tr>
<tr>
<td>Mᵣ</td>
<td>1411.03</td>
</tr>
<tr>
<td>Crystal system, space group</td>
<td>Cubic, Pa 3</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>200</td>
</tr>
<tr>
<td>a, b, c (Å)</td>
<td>24.7459 (2), 24.7459 (2), 24.7459 (2)</td>
</tr>
<tr>
<td>α, β, γ (°)</td>
<td>90, 90, 90</td>
</tr>
<tr>
<td>V (Å³)</td>
<td>15153.4 (4)</td>
</tr>
<tr>
<td>Z</td>
<td>8</td>
</tr>
<tr>
<td>Radiation type</td>
<td>Cu Ka</td>
</tr>
<tr>
<td>μ (mm⁻¹)</td>
<td>6.63</td>
</tr>
<tr>
<td>Crystal size (mm)</td>
<td>0.20 × 0.07 × 0.03</td>
</tr>
<tr>
<td>Diffractometer</td>
<td>SuperNova, Dual, Cu at zero, Atlas</td>
</tr>
<tr>
<td>Absorption correction</td>
<td>Multi-scan</td>
</tr>
<tr>
<td></td>
<td>CrystAlis PRO, Agilent Technologies, Version 1.171.36.28 (release 01-02-2013 CrystAlis171 .NET) (compiled Feb 1 2013,16:14:44)</td>
</tr>
<tr>
<td></td>
<td>Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.</td>
</tr>
<tr>
<td>Tmin, Tmax</td>
<td>0.237, 1.000</td>
</tr>
<tr>
<td>No. of measured, independent and observed [I &gt; 2σ(I)] reflections</td>
<td>19227, 3811, 2602</td>
</tr>
<tr>
<td>Rint</td>
<td>0.057</td>
</tr>
<tr>
<td>θmax (°)</td>
<td>60.9</td>
</tr>
<tr>
<td>sin θλmax, (Å⁻¹)</td>
<td>0.567</td>
</tr>
<tr>
<td>R(F² &gt; 2σ(F²)), wR(F²), S</td>
<td>0.063, 0.174, 1.02</td>
</tr>
<tr>
<td>No. of reflections, parameters, restraints</td>
<td>3811, 229, 18</td>
</tr>
<tr>
<td></td>
<td>w = 1/[σ²(Fo²) + (0.0792P)² + 90.6665P]</td>
</tr>
<tr>
<td></td>
<td>where P = (Fo² + 2Fc²)/3</td>
</tr>
<tr>
<td>Δρmax, Δρmin (e Å⁻³)</td>
<td>1.25, -0.88</td>
</tr>
</tbody>
</table>

Table S2. Summary of gas-phase BS1 and BS2 electronic energies (E_{BS1} and E_{BS2}), thermal correction to Gibbs free energy at the BS1 level (E→G corr.), solvent (PCM) correction at the BS1 level (PCM corr.) and Grimme’s D3(BJ) dispersion correction (D3(BJ) corr.) for all the computed species. All the values are given in Hartrees.

<table>
<thead>
<tr>
<th>Species</th>
<th>E_{BS1}</th>
<th>E_{BS2}</th>
<th>E→G corr.</th>
<th>PCM corr.</th>
<th>D3(BJ) corr.</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₂H₂</td>
<td>-12.4879706</td>
<td>-77.3508384</td>
<td>0.006668</td>
<td>-0.003474626</td>
<td>-0.00194016</td>
</tr>
<tr>
<td>adc</td>
<td>-88.0750677</td>
<td>-454.6361911</td>
<td>0.02127</td>
<td>-0.014955203</td>
<td>-0.0112502</td>
</tr>
<tr>
<td>dmad</td>
<td>-101.836832</td>
<td>-533.25499</td>
<td>0.071176</td>
<td>-0.012476383</td>
<td>-0.01821541</td>
</tr>
<tr>
<td>PhA</td>
<td>-49.0361911</td>
<td>-308.473557</td>
<td>0.07728</td>
<td>-0.004747039</td>
<td>-0.0223392</td>
</tr>
<tr>
<td>bid</td>
<td>-58.3458498</td>
<td>-306.492042</td>
<td>0.05868</td>
<td>-0.018198665</td>
<td>-0.01089777</td>
</tr>
<tr>
<td>PrA</td>
<td>-35.416325</td>
<td>-191.921162</td>
<td>0.031752</td>
<td>-0.0103391</td>
<td>-0.0063206</td>
</tr>
<tr>
<td>EtPr</td>
<td>-64.05917434</td>
<td>-344.6300827</td>
<td>0.064793</td>
<td>-0.008643908</td>
<td>-0.014198</td>
</tr>
<tr>
<td>[1]⁺</td>
<td>-536.087207</td>
<td>-3113.6296</td>
<td>0.4131</td>
<td>-0.06893702</td>
<td>-0.3031083</td>
</tr>
<tr>
<td>TS([1]⁺,C₂H₂)</td>
<td>-548.553584</td>
<td>-3190.96165</td>
<td>0.438719</td>
<td>-0.071176032</td>
<td>-0.32582524</td>
</tr>
<tr>
<td>prod([1]⁺,C₂H₂)</td>
<td>-548.571851</td>
<td>-3190.99135</td>
<td>0.443333</td>
<td>-0.070503058</td>
<td>-0.32849483</td>
</tr>
<tr>
<td>Species</td>
<td>$E_{\text{BS1}}$</td>
<td>$E_{\text{BS2}}$</td>
<td>$E \rightarrow G \text{ corr.}$</td>
<td>PCM corr.</td>
<td>D3(BJ) corr.</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------------</td>
<td>-----------------</td>
<td>--------------------------</td>
<td>----------</td>
<td>-------------</td>
</tr>
<tr>
<td>TS([1]⁺,adc)</td>
<td>-624.147017</td>
<td>-3568.2506</td>
<td>0.457597</td>
<td>-0.079673018</td>
<td>-0.34741347</td>
</tr>
<tr>
<td>prod([1]⁺,adc)</td>
<td>-624.161087</td>
<td>-3568.27472</td>
<td>0.460875</td>
<td>-0.077308925</td>
<td>-0.35227382</td>
</tr>
<tr>
<td>TS([1]⁺,dmad)</td>
<td>-637.906348</td>
<td>-3646.8676</td>
<td>0.507985</td>
<td>-0.077037932</td>
<td>-0.35688909</td>
</tr>
<tr>
<td>prod([1]⁺,dmad)</td>
<td>-637.918593</td>
<td>-3646.89031</td>
<td>0.510196</td>
<td>-0.076259828</td>
<td>-0.36130533</td>
</tr>
<tr>
<td>TS([1]⁺,btd)</td>
<td>-594.416252</td>
<td>-3420.10299</td>
<td>0.49575</td>
<td>-0.077085603</td>
<td>-0.34751198</td>
</tr>
<tr>
<td>prod([1]⁺,btd)</td>
<td>-594.431613</td>
<td>-3420.12884</td>
<td>0.499391</td>
<td>-0.076140404</td>
<td>-0.35181155</td>
</tr>
<tr>
<td>TS([1]⁺,PrA)</td>
<td>-571.481552</td>
<td>-3305.53083</td>
<td>0.465032</td>
<td>-0.077414555</td>
<td>-0.33579774</td>
</tr>
<tr>
<td>prod([1]⁺,PrA)</td>
<td>-571.500823</td>
<td>-3305.56083</td>
<td>0.470321</td>
<td>-0.07493362</td>
<td>-0.33885604</td>
</tr>
<tr>
<td>TS([1]⁺,PhA)</td>
<td>-585.098157</td>
<td>-3422.08075</td>
<td>0.512528</td>
<td>-0.070826058</td>
<td>-0.35959769</td>
</tr>
<tr>
<td>prod([1]⁺,PhA)</td>
<td>-585.114222</td>
<td>-3422.10722</td>
<td>0.516517</td>
<td>-0.070595869</td>
<td>-0.36080795</td>
</tr>
<tr>
<td>TS([2]⁺,C₂H₂)</td>
<td>-600.1285191</td>
<td>-3458.24464</td>
<td>0.494415</td>
<td>-0.07303939</td>
<td>-0.3464422</td>
</tr>
<tr>
<td>prod([2]⁺,C₂H₂)</td>
<td>-600.1440045</td>
<td>-3458.27116</td>
<td>0.503878</td>
<td>-0.07365991</td>
<td>-0.350054</td>
</tr>
<tr>
<td>[2]⁺</td>
<td>-532.849583</td>
<td>-3110.39686</td>
<td>0.412412</td>
<td>-0.06985158</td>
<td>-0.30341216</td>
</tr>
<tr>
<td>TS([2]⁺,ad)</td>
<td>-620.910773</td>
<td>-3565.02039</td>
<td>0.456371</td>
<td>-0.077993582</td>
<td>-0.34819248</td>
</tr>
<tr>
<td>prod([2]⁺,ad)</td>
<td>-620.914644</td>
<td>-3565.03119</td>
<td>0.458112</td>
<td>-0.077997376</td>
<td>-0.35294211</td>
</tr>
<tr>
<td>TS([2]⁺,dmad)</td>
<td>-634.666375</td>
<td>-3643.63324</td>
<td>0.506643</td>
<td>-0.078409654</td>
<td>-0.3580239</td>
</tr>
<tr>
<td>prod([2]⁺,dmad)</td>
<td>-634.675246</td>
<td>-3643.64994</td>
<td>0.508774</td>
<td>-0.074967964</td>
<td>-0.36144826</td>
</tr>
<tr>
<td>TS([2]⁺,btd)</td>
<td>-591.17495</td>
<td>-3416.86706</td>
<td>0.494229</td>
<td>-0.077298253</td>
<td>-0.348737</td>
</tr>
<tr>
<td>prod([2]⁺,btd)</td>
<td>-591.183528</td>
<td>-3416.88431</td>
<td>0.497748</td>
<td>-0.076406507</td>
<td>-0.3525604</td>
</tr>
<tr>
<td>TS([2]⁺,PrA)</td>
<td>-568.241854</td>
<td>-3302.2967</td>
<td>0.465818</td>
<td>-0.076895283</td>
<td>-0.33680437</td>
</tr>
<tr>
<td>prod([2]⁺,PrA)</td>
<td>-568.251399</td>
<td>-3302.31534</td>
<td>0.469456</td>
<td>-0.07543911</td>
<td>-0.33977779</td>
</tr>
<tr>
<td>TS([2]⁺,PhA)</td>
<td>-581.855538</td>
<td>-3418.84338</td>
<td>0.511345</td>
<td>-0.071168434</td>
<td>-0.36073157</td>
</tr>
<tr>
<td>prod([2]⁺,PhA)</td>
<td>-581.865335</td>
<td>-3418.8621</td>
<td>0.51438</td>
<td>-0.070792348</td>
<td>-0.36169705</td>
</tr>
<tr>
<td>TS([2]⁺,EtPr)</td>
<td>-596.8874871</td>
<td>-3455.009404</td>
<td>0.498551</td>
<td>-0.07420785</td>
<td>-0.34733247</td>
</tr>
<tr>
<td>prod([2]⁺,EtPr)</td>
<td>-596.8952115</td>
<td>-3455.026168</td>
<td>0.502425</td>
<td>-0.074336178</td>
<td>-0.35070784</td>
</tr>
</tbody>
</table>
Cartesian coordinates of the DFT-optimised structures

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Cartesian Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₂H₂</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.000000 0.000000 -0.611172</td>
</tr>
<tr>
<td>H</td>
<td>0.000000 0.000000 -1.683748</td>
</tr>
<tr>
<td>C</td>
<td>0.000000 0.000000 0.611172</td>
</tr>
<tr>
<td>H</td>
<td>0.000000 0.000000 1.683749</td>
</tr>
<tr>
<td>adc</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.613250 -0.007104 -0.013114</td>
</tr>
<tr>
<td>C</td>
<td>2.043156 -0.090073 -0.079495</td>
</tr>
<tr>
<td>O</td>
<td>2.648376 0.794167 0.806367</td>
</tr>
<tr>
<td>C</td>
<td>-0.613251 0.006745 -0.013158</td>
</tr>
<tr>
<td>C</td>
<td>-2.043137 0.089912 -0.079495</td>
</tr>
<tr>
<td>O</td>
<td>-2.648562 -0.792713 -0.806466</td>
</tr>
<tr>
<td>O</td>
<td>-2.679562 0.853106 -0.831334</td>
</tr>
<tr>
<td>H</td>
<td>3.636346 0.721099 0.743360</td>
</tr>
<tr>
<td>H</td>
<td>-3.636516 -0.719492 -0.744548</td>
</tr>
<tr>
<td>dmad</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.609694 0.194983 -0.068155</td>
</tr>
<tr>
<td>C</td>
<td>-0.609657 0.193356 0.068610</td>
</tr>
<tr>
<td>C</td>
<td>-2.026774 0.254559 0.288942</td>
</tr>
<tr>
<td>O</td>
<td>-2.586999 0.996033 1.123437</td>
</tr>
<tr>
<td>C</td>
<td>2.027135 0.259262 -0.285526</td>
</tr>
<tr>
<td>O</td>
<td>2.588405 1.011054 -1.110024</td>
</tr>
<tr>
<td>O</td>
<td>2.704381 -0.625080 0.537194</td>
</tr>
<tr>
<td>O</td>
<td>-2.705240 -0.617887 -0.831334</td>
</tr>
<tr>
<td>H</td>
<td>4.188244 -0.639231 0.397867</td>
</tr>
<tr>
<td>H</td>
<td>-4.188999 -0.630250 -0.400998</td>
</tr>
<tr>
<td>EPr</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.067883 -0.552980 0.249488</td>
</tr>
<tr>
<td>C</td>
<td>-1.919570 -0.163034 0.082318</td>
</tr>
<tr>
<td>C</td>
<td>-0.591172 0.354479 -0.102686</td>
</tr>
<tr>
<td>O</td>
<td>-0.272525 1.560403 -0.017400</td>
</tr>
<tr>
<td>C</td>
<td>0.307056 -0.663516 -0.396623</td>
</tr>
<tr>
<td>C</td>
<td>1.742978 -0.260486 -0.603299</td>
</tr>
<tr>
<td>C</td>
<td>2.484799 -0.251657 0.727077</td>
</tr>
<tr>
<td>H</td>
<td>2.110670 -1.032354 -1.291442</td>
</tr>
<tr>
<td>H</td>
<td>1.748236 0.726627 -1.089310</td>
</tr>
<tr>
<td>H</td>
<td>-4.076236 -0.886149 0.397867</td>
</tr>
<tr>
<td>H</td>
<td>3.555115 -0.044549 0.552589</td>
</tr>
<tr>
<td>H</td>
<td>2.090691 0.530742 1.394060</td>
</tr>
<tr>
<td>H</td>
<td>2.400363 -1.227345 1.231025</td>
</tr>
</tbody>
</table>

[1]

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Cartesian Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>PhA</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.523236 -1.217425 0.000058</td>
</tr>
<tr>
<td>C</td>
<td>0.120536 -1.223278 -0.00014</td>
</tr>
<tr>
<td>C</td>
<td>-0.600931 -0.000002 -0.00052</td>
</tr>
<tr>
<td>C</td>
<td>0.120533 1.223277 -0.00017</td>
</tr>
<tr>
<td>C</td>
<td>1.523232 1.217428 0.000055</td>
</tr>
<tr>
<td>C</td>
<td>2.229506 0.000002 0.000996</td>
</tr>
<tr>
<td>H</td>
<td>2.067424 -2.165814 0.000086</td>
</tr>
<tr>
<td>H</td>
<td>-0.431049 -2.166430 -0.000045</td>
</tr>
<tr>
<td>H</td>
<td>-0.431055 2.166427 -0.00050</td>
</tr>
<tr>
<td>H</td>
<td>2.067418 2.165817 0.000081</td>
</tr>
<tr>
<td>H</td>
<td>3.322758 0.000004 0.001516</td>
</tr>
<tr>
<td>H</td>
<td>-2.032813 -0.000003 -0.000164</td>
</tr>
<tr>
<td>H</td>
<td>-3.260497 -0.000003 -0.000106</td>
</tr>
<tr>
<td>H</td>
<td>-4.332313 0.000023 0.000630</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Cartesian Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>PrA</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-2.973780 -0.559764 -0.000082</td>
</tr>
<tr>
<td>C</td>
<td>-1.954297 -0.229312 -0.000042</td>
</tr>
<tr>
<td>C</td>
<td>-0.791543 0.150705 0.000027</td>
</tr>
<tr>
<td>C</td>
<td>0.594637 0.605515 0.000019</td>
</tr>
<tr>
<td>O</td>
<td>1.483620 -0.589887 0.000104</td>
</tr>
<tr>
<td>H</td>
<td>0.792277 1.220632 -0.896098</td>
</tr>
</tbody>
</table>
\[ \text{prod}([\text{I}], \text{adc}) \]

\[
\begin{align*}
\text{N} &: -2.771193 -2.035026 -1.249395 \\
\text{C} &: 3.929274 -2.470553 -0.622618 \\
\text{C} &: 4.695732 -3.505309 -1.181552 \\
\text{C} &: 4.311426 -4.096484 -2.392145 \\
\text{C} &: 3.153958 -3.633477 -3.030837 \\
\text{C} &: 2.412691 -2.607448 -2.434486 \\
\text{C} &: 4.294119 -1.787584 0.623901 \\
\text{N} &: 3.429307 -0.811504 1.067533 \\
\text{C} &: 3.719202 -0.145578 2.220329 \\
\text{C} &: 4.872702 -0.413412 2.968567 \\
\text{C} &: 5.765886 -1.396348 2.521121 \\
\text{C} &: 5.468846 -2.087958 1.359956 \\
\text{Mo} &: 1.643518 -0.411569 -0.226768
\end{align*}
\]

\[
\begin{align*}
\text{O} &: -0.902888 -1.417439 -0.399466 \\
\text{Cl} &: -0.524523 -3.556830 -1.563395 \\
\text{N} &: 2.792690 -1.476047 -1.614321 \\
\text{C} &: -3.879483 -2.102057 -1.036107 \\
\text{C} &: -5.124109 -2.129192 -1.690313 \\
\text{C} &: -5.261062 -1.554241 -2.962374 \\
\text{C} &: -4.139963 -0.971002 -3.564450 \\
\text{C} &: -2.928888 -0.941198 -2.860926 \\
\text{C} &: -3.635998 -2.793079 0.240335 \\
\text{C} &: -4.632828 -3.536890 0.930132 \\
\text{C} &: -4.323118 -4.245078 2.069591 \\
\text{C} &: -3.006509 -4.207215 2.551074 \\
\text{C} &: -2.056079 -3.442207 1.866873 \\
\text{C} &: -2.353636 -2.731513 0.742196 \\
\text{H} &: 0.234448 -0.245892 -2.221266 \\
\text{S} &: 0.661777 -1.853599 1.347224 \\
\text{H} &: -1.215215 3.400283 0.203481 \\
\text{C} &: -0.595033 4.518560 -0.308366 \\
\text{C} &: -0.923363 5.803735 0.168302 \\
\text{H} &: -1.902098 5.957628 1.157005 \\
\text{C} &: -2.554091 4.815599 1.645196 \\
\text{C} &: -2.186755 3.561245 1.147221 \\
\text{C} &: 0.361300 4.291556 -1.400422 \\
\text{H} &: 1.044847 5.341637 -2.040590 \\
\text{C} &: 1.867523 5.075526 -3.140378 \\
\text{H} &: 1.982184 3.753463 -3.590891 \\
\text{C} &: 1.304651 2.739081 -2.904815 \\
\text{H} &: 0.516565 2.983071 1.817300 \\
\text{C} &: 3.390421 0.99904-1.330050 \\
\text{H} &: 0.930090 6.367102 -1.689951 \\
\text{C} &: 1.835406 1.704316 -3.219080 \\
\text{H} &: -0.426012 6.683641 -0.238831 \\
\text{C} &: -2.682634 2.657920 1.491797 \\
\text{C} &: 2.598558 3.493288 -4.452262 \\
\text{C} &: -3.337607 4.882964 2.400995 \\
\text{C} &: 5.597985 -3.848979 -0.676705 \\
\text{C} &: 1.513987 -2.223264 -2.904655 \\
\text{H} &: 6.154626 -2.853720 0.977808 \\
\text{C} &: 3.013430 0.607734 2.561986 \\
\text{H} &: 2.813610 -4.056265 -3.976796 \\
\text{C} &: 5.048619 0.151782 3.844499 \\
\text{H} &: -5.647182 -3.571076 0.506768 \\
\text{H} &: -1.026318 -3.387242 2.211129 \\
\text{C} &: -5.983792 -2.607852 -1.221990 \\
\text{C} &: -2.038842 -0.496220 -3.292857 \\
\text{C} &: -2.709512 -4.758358 3.444464 \\
\text{C} &: -4.190656 -0.525460 -4.558501 \\
\text{H} &: 4.909769 -4.899281 -2.827163 \\
\text{C} &: 6.676978 -1.623818 3.077816 \\
\text{C} &: -6.225225 -1.573582 -3.473889 \\
\text{C} &: -5.093520 -4.821506 2.585084 \\
\text{C} &: 2.398411 5.887187 -3.643915 \\
\text{C} &: -2.158394 6.951630 1.528362 \\
\text{C} &: 0.750723 1.710695 3.963872 \\
\text{C} &: -1.850279 -0.047162 3.798050 \\
\text{O} &: -1.034609 -0.527624 4.823080 \\
\text{C} &: -3.093483 -0.142999 3.832651 \\
\text{C} &: -1.593030 -0.859808 5.572760 \\
\text{H} &: -0.119404 2.318969 4.684489 \\
\text{C} &: 1.985237 1.653569 4.163052
\end{align*}
\]
TS([1]^+PhA)
N 2.684878 2.501325 -0.611575
C 3.000253 3.647369 0.086867
C 4.249872 2.729293 -0.079019
C 5.183017 3.754634 -0.981826
C 4.841945 2.599189 -1.710587
C 3.591860 2.004354 -1.499010
C 1.951419 4.185919 0.964959
N 0.762603 3.490559 1.020702
C -0.258807 3.978862 1.761433
C -0.146061 5.150575 2.516878
C 1.066390 5.856133 2.499753
C 2.117204 5.360767 1.714903
Mo 0.654095 1.620582 -0.232017
S 1.044147 -0.009522 -2.010782
Mo -1.087125 -0.526355 -0.934952
S -0.624889 -1.990812 0.898640
Mo 0.148605 -1.139750 0.119308
Cl 3.898405 -0.910574 -0.212587
N 1.846375 -3.066664 -0.985955
C 2.314581 -4.096226 -0.241545
C 2.603621 -5.332144 -0.848312
C 2.430120 -5.492597 -2.230080
C 1.972532 -4.404693 -2.983686
C 1.689354 -3.197049 -2.333290
C 2.502927 -3.845303 1.192323
N 2.202026 -2.584772 1.645574
C 2.401784 -2.288755 2.960378
C 2.914108 -3.216033 3.873167
C 3.236415 -4.050735 3.423184
C 3.037039 -4.816917 0.723826
S 1.474860 0.654489 1.777035
S -1.573724 1.314491 0.508782
Cl 0.071583 3.338055 -1.947648
Cl -1.410456 -2.418724 -2.532638
N -2.172096 0.517413 -2.610396
C -3.546590 0.407021 -2.615611
C -4.312376 1.025513 -3.620997
C -3.677803 1.744740 -4.643573
C -2.279926 1.826227 -4.645135
C -1.561635 1.203946 -3.616044
C -4.145147 -0.408412 -1.547740
C -5.531124 -0.651412 -1.465777
C -6.044756 -1.459922 -0.441081
C -5.157599 -2.001157 0.495516
C -3.789126 -1.729848 0.373031
N -3.279160 -0.954924 -0.625213
C -1.372473 0.520794 2.969158
C -0.135049 0.576401 3.286439
H 0.465199 0.654065 4.188668
H 4.495492 5.173825 0.483173
N 3.299096 1.111147 -2.041230
H 3.061382 5.911002 1.681166
H -1.180682 3.404022 1.745077
H 5.529450 2.153938 -2.430764
H -0.998417 5.495515 3.104048
H 2.969469 -6.167245 -0.251309
H 1.303690 -2.334659 -2.885166
H 3.290685 -5.811377 1.706885
H 2.147867 -1.276951 3.262492
H 1.824780 -4.476961 -0.401836
H 3.059644 -2.933536 4.914019
H -6.208201 -0.223137 -2.204461
H -3.069586 -2.132494 1.079840
H -5.399094 0.944490 -3.615943
H -0.478119 1.245480 -3.584872
H -5.504872 -2.628609 1.316229
H -1.738562 2.368338 -5.421511
H 2.655056 -6.449360 -2.705250
H 3.640340 -5.254171 4.107477
H -4.268632 2.224822 -5.426108
H -7.117142 -1.645817 -0.378321
H 6.152992 4.228334 -1.156644
H 1.190907 6.772457 3.079950
H -2.732896 0.256248 3.360813
H -3.024779 -0.994679 1.063772
H -3.788662 1.175696 3.118122
H -3.422471 -1.206066 4.522471
H -2.219141 -1.665004 4.244915
H -5.082920 0.911644 3.589760
H -3.582826 2.092921 2.562177
H -5.358480 -0.277200 4.292003
H -4.529335 -2.128650 5.072460
H -5.880519 1.637236 3.409897
H -6.376955 -0.476398 4.660415
prod([1]^+PhA)
N 1.881475 2.998524 -0.857420
C 1.897137 4.233800 -0.232697
C 2.964176 5.132248 -0.420790
C 4.017176 4.804945 -1.283580
C 3.973011 3.574661 -1.952896
C 2.907051 2.702156 -1.712276
C 0.717611 4.569745 0.51892
N  -0.274274  3.616032  0.625162
C  -1.438272  3.915466  1.269046
C  -1.652132  5.137132  1.914831
C  -0.630833  6.099623  1.901720
C   0.555260  5.813053  1.217702
Mo  0.180139  1.650897  -0.399094
S   1.073937  0.077779  -2.009435
Mo  -0.825844  -0.969298  -0.881564
S   -0.047583  -2.078953  1.093739
Mo  1.670613  -0.723414  0.222435
Cl  3.937466   0.311801  0.033844
N   2.692306  -2.453306  -0.734686
C   3.386911  -3.300127  0.107493
C   4.009306  -4.458255  -0.392175
C   3.946893  -4.755388  -1.760718
C   3.263186  -3.877586  -2.610498
C   2.647456  -2.743912  -2.065780
C   3.468212  -2.901234  1.520024
N   2.796903  -1.752126  1.869300
C   2.882256  -1.303584  3.152742
C   3.610535  -1.976866  4.319282
C   4.285110  -3.158988  3.790506
C   4.214405  -3.617777  2.747746
S   1.049746  1.151614  1.809698
Mo  -0.825844  -0.969298  -0.881564
S   -0.047583  -2.078953  1.093739
Mo  1.670613  -0.723414  0.222435
Cl  3.937466   0.311801  0.033844
N   2.692306  -2.453306  -0.734686
C   3.386911  -3.300127  0.107493
C   4.009306  -4.458255  -0.392175
C   3.946893  -4.755388  -1.760718
C   3.263186  -3.877586  -2.610498
C   2.647456  -2.743912  -2.065780
C   3.468212  -2.901234  1.520024
N   2.796903  -1.752126  1.869300
prod([2]+C2H2)
N 0.574120 3.130145 -1.163031
C 0.560538 4.398210 0.924309
C 1.272621 5.454848 1.620171
C 1.981149 5.243467 -2.393241
C 1.951461 3.970353 -2.975807
C -0.276330 4.579331 0.586783
C -0.448013 5.830822 1.213869
C -1.297863 5.954614 2.317748
C -1.975873 4.814559 2.770724
C -1.770125 3.594806 2.125885
N -0.932506 3.459591 1.056028
W -0.527582 1.529276 -0.053409
S 1.395736 1.499631 1.566371
W 1.591900 -0.365181 -0.078317
N 3.512041 -0.956066 0.962172
C 4.107301 -2.114939 0.513588
C 5.283783 -2.600701 1.121158
C 5.876970 -1.892318 2.170916
C 5.289005 -0.687334 2.588603
C 4.117020 -0.253817 1.964445
C 3.484189 -2.753907 -0.648427
C 4.007433 -3.917256 -1.241663

prod([2]+C2H2)
N 3.442701 -4.426602 -2.416898
C 2.358206 -3.743270 -2.984178
C 1.850384 -2.609487 -2.344507
N 2.374998 -2.111209 -1.181018
W -1.153564 -1.139196 0.010553
N -2.623044 -2.404868 1.144873
C -3.896499 -2.467107 0.623960
C -4.898424 -3.224948 1.261589
C -6.052621 -3.913669 2.433902
C -3.300327 -3.876418 2.946022
C -2.341033 -3.109599 2.276855
C -4.122916 -1.736118 -0.631195
C -5.375386 -1.698827 -1.272116
C -5.516542 -1.039860 -2.501003
C -4.392142 -0.433622 -3.073844
C -3.169846 -0.483406 -2.393585
N -3.023549 -1.107047 -1.188781
C -0.890120 -3.386132 -1.084178
S -0.021701 -0.042362 -1.895430
S 0.659963 -1.796049 1.670051
C -2.403456 2.420556 -1.430753
C 3.323310 0.881032 -1.402664
C 4.866298 -4.419841 -0.796817
C 1.005194 -2.070637 -2.756930
C 5.743586 -3.522370 0.765642
C 3.642795 0.681588 2.246741
C 1.899730 -4.083317 -3.980663
C 5.703063 -0.384302 3.381367
C -6.236907 -2.186033 -0.819686
C -2.278651 -0.026215 -2.809753
C -5.902577 -3.273000 0.841210
C -1.313453 -3.057560 2.625329
C -4.446544 0.084938 -0.431661
C -3.018351 -4.423353 3.846874
C 0.071596 6.709961 0.833961
C -2.279496 2.689301 2.446196
C 1.268624 6.447570 -0.748546
C 1.198369 1.949084 -2.767991
C -2.662518 4.861256 3.623509
C 2.471680 3.756577 -3.910173
C -6.486967 -1.096064 -2.999393
C -5.378839 -4.521340 2.929908
C 2.533397 6.062054 -2.858545
C -1.435255 6.923315 2.802062
C 3.848235 -5.326953 -2.881737
C 6.788308 -2.265307 2.642151
C 0.601243 -0.698235 3.237315
C 0.307914 -1.244756 4.136187
C 0.903141 0.594906 3.198704
C 0.879534 1.271556 4.054899

TS([2]+adc)
N 3.446432 -0.681161 1.113372
C 4.365886 -1.537460 0.541916
C 5.520741 -1.928212 1.247584
C 5.745851 -1.454984 2.543383
C 4.795958 -0.600874 3.124418
C 3.664462 -0.240160 2.385795
C 4.072030 -2.006086 -0.820681
<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>2.921384</td>
<td>-1.516897</td>
<td>-1.405800</td>
</tr>
<tr>
<td>C</td>
<td>2.620797</td>
<td>-1.888241</td>
<td>-2.682249</td>
</tr>
<tr>
<td>C</td>
<td>3.426238</td>
<td>-2.765224</td>
<td>-3.418349</td>
</tr>
<tr>
<td>C</td>
<td>4.586096</td>
<td>-2.821374</td>
<td>-2.713070</td>
</tr>
<tr>
<td>C</td>
<td>4.909021</td>
<td>-2.895086</td>
<td>-1.905265</td>
</tr>
<tr>
<td>W</td>
<td>1.699620</td>
<td>-0.082423</td>
<td>-0.175252</td>
</tr>
<tr>
<td>Cl</td>
<td>3.463063</td>
<td>1.433902</td>
<td>-1.103627</td>
</tr>
<tr>
<td>W</td>
<td>-0.867914</td>
<td>-1.199584</td>
<td>-0.682270</td>
</tr>
<tr>
<td>Cl</td>
<td>-0.357249</td>
<td>-3.026747</td>
<td>-2.324651</td>
</tr>
<tr>
<td>N</td>
<td>-2.681427</td>
<td>-1.105085</td>
<td>-2.006539</td>
</tr>
<tr>
<td>C</td>
<td>-3.721822</td>
<td>-1.957617</td>
<td>-1.699974</td>
</tr>
<tr>
<td>C</td>
<td>-4.905282</td>
<td>-1.948601</td>
<td>-2.460351</td>
</tr>
<tr>
<td>C</td>
<td>-5.026829</td>
<td>-1.085325</td>
<td>-3.557881</td>
</tr>
<tr>
<td>C</td>
<td>-3.951175</td>
<td>-0.248775</td>
<td>-3.882135</td>
</tr>
<tr>
<td>W</td>
<td>1.699620</td>
<td>-0.082423</td>
<td>-0.175252</td>
</tr>
<tr>
<td>Cl</td>
<td>3.463063</td>
<td>1.433902</td>
<td>-1.103627</td>
</tr>
<tr>
<td>W</td>
<td>-0.867914</td>
<td>-1.199584</td>
<td>-0.682270</td>
</tr>
<tr>
<td>Cl</td>
<td>-0.357249</td>
<td>-3.026747</td>
<td>-2.324651</td>
</tr>
<tr>
<td>N</td>
<td>-2.681427</td>
<td>-1.105085</td>
<td>-2.006539</td>
</tr>
<tr>
<td>C</td>
<td>-3.721822</td>
<td>-1.957617</td>
<td>-1.699974</td>
</tr>
<tr>
<td>C</td>
<td>-4.905282</td>
<td>-1.948601</td>
<td>-2.460351</td>
</tr>
<tr>
<td>C</td>
<td>-5.026829</td>
<td>-1.085325</td>
<td>-3.557881</td>
</tr>
<tr>
<td>C</td>
<td>-3.951175</td>
<td>-0.248775</td>
<td>-3.882135</td>
</tr>
</tbody>
</table>

prod([2],adc)

N  2.500938  -2.307736  -1.228648
C  3.629505  -2.844341  -0.636446
C  4.283282  -3.949416  -1.211033
C  3.801606  -4.513574  -2.399439
C  2.666785  -3.953634  -3.000105
C  2.046461  -2.856995  -2.397284
C  4.095633  -2.196028  0.596506
C  3.305373  -1.146923  1.061698
C  3.704144  -0.521841  2.214896
C  4.844574  -0.898330  2.953057
C  5.639244  -1.950704  2.461011
C  5.254616  -2.604032  1.283211
C  1.570619  -0.567996  -0.204034
C  1.275406  1.522877  1.747575
C  0.250674  1.232687  2.883345
C  -0.924743  0.608496  2.828061
C  -1.990864  0.566354  1.097253
C  -0.396070  1.482698  -0.555927
C  -2.230842  2.316132  -0.054828
C  -1.085960  -1.274685  -0.328518
C  -0.978712  -3.455405  -1.508855
C  -2.982089  -1.109054  -1.512111
C  -4.125590  -1.620011  -0.925245
C  -5.373965  -1.501257  -1.560662
C  -5.465313  -0.891248  -2.823628
C  -4.295078  -0.433495  -3.435209
C  -3.078084  -0.546828  -2.751952
C  -3.942821  -2.348017  0.339986
C  -5.004488  -2.988165  1.008910
C  -4.757521  -3.737695  2.164531
C  -3.438437  -3.846020  2.627629
C  -2.420157  -3.180298  1.938383
C  -2.653883  -2.429278  0.824310
C  -0.153198  -0.246244  -2.207072
C  -0.458219  -1.914101  1.408082
C  -0.833009  3.523283  0.312930
C  -0.105527  4.572415  -0.207251
C  -0.281048  5.881383  0.283161
C  -1.214019  6.133593  1.295643
C  -1.974437  5.065471  1.793927
C  -1.758982  3.782554  1.281070
C  -0.797396  4.250169  -1.320288
C  1.582794  5.221417  -1.966371
C  2.348846  4.874958  -3.087446
C  2.303960  3.553080  -3.547730
prod([2] \cdot btd)

N 0.813174 -2.918362 -1.645582
C 1.496098 -4.058428 -1.251643
C 1.347576 -5.273234 -1.947649
<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1.874658</td>
<td>-4.477472</td>
<td>-3.956842</td>
</tr>
<tr>
<td>H</td>
<td>3.206356</td>
<td>-2.721584</td>
<td>4.964745</td>
</tr>
<tr>
<td>H</td>
<td>-6.260028</td>
<td>1.161866</td>
<td>-3.541102</td>
</tr>
<tr>
<td>H</td>
<td>-3.011508</td>
<td>-2.225170</td>
<td>1.218161</td>
</tr>
<tr>
<td>H</td>
<td>-5.513372</td>
<td>0.663374</td>
<td>-3.509111</td>
</tr>
<tr>
<td>H</td>
<td>-0.608562</td>
<td>1.161866</td>
<td>-3.541102</td>
</tr>
<tr>
<td>H</td>
<td>-5.424282</td>
<td>-2.791377</td>
<td>1.505957</td>
</tr>
<tr>
<td>H</td>
<td>2.760344</td>
<td>-6.407514</td>
<td>-2.574457</td>
</tr>
<tr>
<td>H</td>
<td>3.809803</td>
<td>-5.061157</td>
<td>4.200575</td>
</tr>
<tr>
<td>H</td>
<td>-4.456342</td>
<td>1.967879</td>
<td>-5.346506</td>
</tr>
<tr>
<td>H</td>
<td>-7.093724</td>
<td>-1.915335</td>
<td>-0.190311</td>
</tr>
<tr>
<td>H</td>
<td>5.922442</td>
<td>4.434520</td>
<td>-1.246881</td>
</tr>
<tr>
<td>H</td>
<td>0.930763</td>
<td>6.858540</td>
<td>3.007671</td>
</tr>
<tr>
<td>C</td>
<td>-2.800732</td>
<td>0.290261</td>
<td>3.410387</td>
</tr>
<tr>
<td>C</td>
<td>-3.048573</td>
<td>-0.892631</td>
<td>4.661462</td>
</tr>
<tr>
<td>C</td>
<td>-3.838030</td>
<td>1.173878</td>
<td>3.158014</td>
</tr>
<tr>
<td>H</td>
<td>-2.222215</td>
<td>-1.583369</td>
<td>3.451764</td>
</tr>
<tr>
<td>C</td>
<td>-5.160826</td>
<td>0.896562</td>
<td>3.668940</td>
</tr>
<tr>
<td>C</td>
<td>-7.133382</td>
<td>2.074540</td>
<td>5.263624</td>
</tr>
<tr>
<td>C</td>
<td>-3.927894</td>
<td>-0.268736</td>
<td>4.420358</td>
</tr>
<tr>
<td>H</td>
<td>-4.502245</td>
<td>-2.070882</td>
<td>5.248851</td>
</tr>
<tr>
<td>H</td>
<td>-5.979159</td>
<td>1.598768</td>
<td>3.480450</td>
</tr>
<tr>
<td>H</td>
<td>-6.389115</td>
<td>-0.477695</td>
<td>4.818111</td>
</tr>
<tr>
<td>prod([2]+PhA)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>1.879279</td>
<td>2.950889</td>
<td>-0.842097</td>
</tr>
<tr>
<td>C</td>
<td>1.937483</td>
<td>4.189564</td>
<td>-0.219868</td>
</tr>
<tr>
<td>C</td>
<td>3.025160</td>
<td>5.058432</td>
<td>-0.424109</td>
</tr>
<tr>
<td>C</td>
<td>4.057402</td>
<td>4.704250</td>
<td>-1.300911</td>
</tr>
<tr>
<td>C</td>
<td>3.969666</td>
<td>3.745250</td>
<td>-0.962790</td>
</tr>
<tr>
<td>C</td>
<td>2.888249</td>
<td>2.630629</td>
<td>-1.713954</td>
</tr>
<tr>
<td>C</td>
<td>0.780451</td>
<td>4.556383</td>
<td>0.601195</td>
</tr>
<tr>
<td>N</td>
<td>-0.231892</td>
<td>3.623481</td>
<td>0.676311</td>
</tr>
<tr>
<td>C</td>
<td>-1.378889</td>
<td>3.954307</td>
<td>1.336963</td>
</tr>
<tr>
<td>C</td>
<td>-1.558343</td>
<td>5.182944</td>
<td>1.979798</td>
</tr>
<tr>
<td>C</td>
<td>-0.511320</td>
<td>6.122290</td>
<td>1.945432</td>
</tr>
<tr>
<td>C</td>
<td>0.659572</td>
<td>5.080828</td>
<td>1.243231</td>
</tr>
<tr>
<td>W</td>
<td>0.164275</td>
<td>1.644810</td>
<td>-0.346801</td>
</tr>
<tr>
<td>S</td>
<td>0.999251</td>
<td>0.054520</td>
<td>-2.015992</td>
</tr>
<tr>
<td>Cl</td>
<td>-0.922170</td>
<td>-0.935049</td>
<td>-0.811412</td>
</tr>
<tr>
<td>N</td>
<td>-0.138048</td>
<td>-2.079762</td>
<td>1.172936</td>
</tr>
<tr>
<td>W</td>
<td>1.606387</td>
<td>-0.748467</td>
<td>0.241163</td>
</tr>
<tr>
<td>Cl</td>
<td>0.314802</td>
<td>0.216385</td>
<td>-0.017267</td>
</tr>
<tr>
<td>N</td>
<td>2.561482</td>
<td>-2.505420</td>
<td>-0.726692</td>
</tr>
<tr>
<td>C</td>
<td>3.260143</td>
<td>-3.633322</td>
<td>0.104014</td>
</tr>
<tr>
<td>C</td>
<td>3.841776</td>
<td>-4.538846</td>
<td>-0.402432</td>
</tr>
<tr>
<td>C</td>
<td>3.734223</td>
<td>-4.847325</td>
<td>1.165559</td>
</tr>
<tr>
<td>C</td>
<td>3.046167</td>
<td>-3.961745</td>
<td>-2.603541</td>
</tr>
<tr>
<td>C</td>
<td>2.473208</td>
<td>-2.808876</td>
<td>2.054113</td>
</tr>
<tr>
<td>C</td>
<td>3.383123</td>
<td>-2.959806</td>
<td>1.511911</td>
</tr>
<tr>
<td>N</td>
<td>2.741205</td>
<td>-1.795344</td>
<td>1.871082</td>
</tr>
<tr>
<td>C</td>
<td>2.857205</td>
<td>-1.351094</td>
<td>3.154616</td>
</tr>
<tr>
<td>C</td>
<td>3.587864</td>
<td>-2.039834</td>
<td>4.128006</td>
</tr>
<tr>
<td>C</td>
<td>4.234617</td>
<td>-3.233870</td>
<td>3.775412</td>
</tr>
<tr>
<td>C</td>
<td>4.131569</td>
<td>-3.690107</td>
<td>2.456100</td>
</tr>
<tr>
<td>S</td>
<td>1.065695</td>
<td>1.137922</td>
<td>1.862629</td>
</tr>
<tr>
<td>S</td>
<td>-1.976423</td>
<td>0.869677</td>
<td>0.561633</td>
</tr>
<tr>
<td>Cl</td>
<td>-0.958030</td>
<td>2.970250</td>
<td>-2.167863</td>
</tr>
<tr>
<td>prod([2]+EtPr)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>1.694661</td>
<td>3.030338</td>
<td>-1.041261</td>
</tr>
<tr>
<td>C</td>
<td>1.631355</td>
<td>4.307503</td>
<td>-0.522091</td>
</tr>
<tr>
<td>C</td>
<td>2.625684</td>
<td>5.256142</td>
<td>-0.822637</td>
</tr>
<tr>
<td>C</td>
<td>3.682607</td>
<td>4.918162</td>
<td>-1.678544</td>
</tr>
<tr>
<td>C</td>
<td>3.718965</td>
<td>3.630807</td>
<td>-2.229496</td>
</tr>
<tr>
<td>C</td>
<td>2.715870</td>
<td>2.716350</td>
<td>-1.888757</td>
</tr>
<tr>
<td>Cl</td>
<td>0.458122</td>
<td>4.617978</td>
<td>0.307922</td>
</tr>
</tbody>
</table>

TS([2]+EtPr)