

Supporting Information for  
**Are Disulfide Bonds Resilient to Double Ionization? Insights from Coincidence  
Spectroscopy and Ab Initio Calculations**

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## Electronic Energy and Thermochemical Analysis

**Table S1.** Electronic energies and thermochemical analysis of **1a** and **1b**. All values are in Hartree.

<b>M06-2X/cc-pVTZ</b>	<b>1a</b>	<b>1b</b>
Electronic energy	-875.40466	-875.40285
Zero-point correction	0.07396	0.07385
Thermal correction to energy	0.07975	0.07974
Thermal correction to enthalpy	0.08069	0.08069
Thermal correction to Gibbs free energy	0.04420	0.04377
Sum of electronic and zero-point energies	-875.33070	-875.32900
Sum of electronic and thermal energies	-875.32491	-875.32310
Sum of electronic and thermal enthalpies	-875.32397	-875.32216
Sum of electronic and thermal free energies	-875.36046	-875.35908
<b>CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ</b>	<b>1a</b>	<b>1b</b>
Electronic energy	-874.38423	-874.38253

**Table S2.** Electronic energies and thermochemical analysis of **2a** and **2b**. All values are in Hartree.

<b>M06-2X/cc-pVTZ</b>	<b>2a</b>	<b>2b</b>
Electronic energy	-875.39660	-875.39320
Zero-point correction	0.07144	0.07134
Thermal correction to energy	0.07768	0.07762
Thermal correction to enthalpy	0.07862	0.07856
Thermal correction to Gibbs free energy	0.04152	0.04136
Sum of electronic and zero-point energies	-875.32517	-875.32186
Sum of electronic and thermal energies	-875.31893	-875.31559
Sum of electronic and thermal enthalpies	-875.31798	-875.31464
Sum of electronic and thermal free energies	-875.35509	-875.35184
<b>CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ</b>	<b>2a</b>	<b>2b</b>
Electronic energy	-874.37413	-874.37075

**Table S3.** Electronic energies and thermochemical analysis of **3** and **4**. All values are in Hartree.

<b>M06-2X/cc-pVTZ</b>	<b>3</b>	<b>4</b>
Electronic energy	-875.39089	-875.39196
Zero-point correction	0.07142	0.07428
Thermal correction to energy	0.07749	0.08035
Thermal correction to enthalpy	0.07843	0.08129
Thermal correction to Gibbs free energy	0.04149	0.04370

Sum of electronic and zero-point energies	-875.31947	-875.31768
Sum of electronic and thermal energies	-875.31340	-875.31161
Sum of electronic and thermal enthalpies	-875.31246	-875.31067
Sum of electronic and thermal free energies	-875.34940	-875.34826
<b>CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ</b>	<b>3</b>	<b>4</b>
Electronic energy	-874.36842	-874.37116

**Table S4.** Electronic energies and thermochemical analysis of **5** and **6**. All values are in Hartree.

<b>M06-2X/cc-pVTZ</b>	<b>5</b>	<b>6</b>
Electronic energy	-875.39172	-875.38166
Zero-point correction	0.07426	0.07715
Thermal correction to energy	0.07964	0.08188
Thermal correction to enthalpy	0.08058	0.08283
Thermal correction to Gibbs free energy	0.04528	0.04896
Sum of electronic and zero-point energies	-875.31747	-875.30451
Sum of electronic and thermal energies	-875.31209	-875.29978
Sum of electronic and thermal enthalpies	-875.31115	-875.29883
Sum of electronic and thermal free energies	-875.34645	-875.33270
<b>CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ</b>	<b>5</b>	<b>6</b>
Electronic energy	-874.36600	-874.35971

**Table S5.** Electronic energies and thermochemical analysis of **7** and **8**. All values are in Hartree.

<b>M06-2X/cc-pVTZ</b>	<b>7</b>	<b>8</b>
Electronic energy	-875.37879	-875.37943
Zero-point correction	0.07337	0.07423
Thermal correction to energy	0.07980	0.08031
Thermal correction to enthalpy	0.08075	0.08126
Thermal correction to Gibbs free energy	0.04296	0.04424
Sum of electronic and zero-point energies	-875.30542	-875.30519
Sum of electronic and thermal energies	-875.29898	-875.29912
Sum of electronic and thermal enthalpies	-875.29804	-875.29817
Sum of electronic and thermal free energies	-875.33582	-875.33518
<b>CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ</b>	<b>7</b>	<b>8</b>
Electronic energy	-874.35719	-874.35744

**Table S6.** Electronic energies and thermochemical analysis of **9** and **10**. All values are in Hartree.

<b>M06-2X/cc-pVTZ</b>	<b>9</b>	<b>10</b>
Electronic energy	-875.37877	-875.38059
Zero-point correction	0.07497	0.07530
Thermal correction to energy	0.08123	0.08090
Thermal correction to enthalpy	0.08217	0.08184
Thermal correction to Gibbs free energy	0.04461	0.04633
Sum of electronic and zero-point energies	-875.30380	-875.30530
Sum of electronic and thermal energies	-875.29755	-875.29970
Sum of electronic and thermal enthalpies	-875.29660	-875.29875
Sum of electronic and thermal free energies	-875.33417	-875.33426
<b>CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ</b>	<b>9</b>	<b>10</b>
Electronic energy	-874.35545	-874.35355

**Table S7.** Electronic energies and thermochemical analysis of **11** and **12**. All values are in Hartree.

<b>M06-2X/cc-pVTZ</b>	<b>11</b>	<b>12</b>
Electronic energy	-875.37208	-875.37330
Zero-point correction	0.07723	0.07644
Thermal correction to energy	0.08212	0.08193
Thermal correction to enthalpy	0.08306	0.08287
Thermal correction to Gibbs free energy	0.04888	0.04762
Sum of electronic and zero-point energies	-875.29484	-875.29687
Sum of electronic and thermal energies	-875.28996	-875.29137
Sum of electronic and thermal enthalpies	-875.28901	-875.29043
Sum of electronic and thermal free energies	-875.32319	-875.32568
<b>CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ</b>	<b>11</b>	<b>12</b>
Electronic energy	-874.34933	-874.34656

**Table S8.** Electronic energies and thermochemical analysis of **13** and **14**. All values are in Hartree.

<b>M06-2X/cc-pVTZ</b>	<b>13</b>	<b>14</b>
Electronic energy	-875.36175	-875.35834
Zero-point correction	0.07552	0.07532
Thermal correction to energy	0.08196	0.08064
Thermal correction to enthalpy	0.08291	0.08158
Thermal correction to Gibbs free energy	0.04538	0.04672
Sum of electronic and zero-point energies	-875.28623	-875.28302
Sum of electronic and thermal energies	-875.27979	-875.27770

Sum of electronic and thermal enthalpies	-875.27884	-875.27676
Sum of electronic and thermal free energies	-875.31637	-875.31162
<b>CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ</b>	<b>13</b>	<b>14</b>
Electronic energy	-874.33783	-874.33310

**Table S9.** Relative enthalpies at the M06-2X/cc-pVTZ (DFT) and CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ (CC) levels of theory.

Species	H (DFT), Hartree	$\Delta H$ (DFT), kcal mol <sup>-1</sup>	H (CC), Hartree	$\Delta H$ (CC), kcal mol <sup>-1</sup>
<b>1a</b>	-875.32397	0.0	-874.30354	0.0
<b>1b</b>	-875.32216	1.1	-874.30185	1.1
<b>2a</b>	-875.31798	3.8	-874.29551	5.0
<b>2b</b>	-875.31464	5.9	-874.29218	7.1
<b>3</b>	-875.31246	7.2	-874.28999	8.5
<b>4</b>	-875.31067	8.3	-874.28987	8.6
<b>5</b>	-875.31114	8.0	-874.28542	11.4
<b>6</b>	-875.29883	15.8	-874.27689	16.7
<b>7</b>	-875.29804	16.3	-874.27644	17.0
<b>8</b>	-875.29817	16.2	-874.27618	17.2
<b>9</b>	-875.29660	17.2	-874.27328	19.0
<b>10</b>	-875.29875	15.8	-874.27171	20.0
<b>11</b>	-875.28901	21.9	-874.26627	23.4
<b>12</b>	-875.29043	21.0	-874.26369	25.0
<b>13</b>	-875.27884	28.3	-874.25492	30.5
<b>14</b>	-875.27676	29.6	-874.25152	32.6

## Cartesian Coordinates

### **1a (M06-2X/cc-pVTZ)**

S	-2.062130000	-0.235728000	-0.085624000
C	-0.466186000	0.637702000	0.266799000
C	0.676896000	-0.318666000	0.388319000
S	2.141927000	0.059778000	-0.200958000
H	-2.069573000	-0.156736000	-1.439204000
H	-2.884132000	0.827850000	0.099902000
H	-0.306384000	1.439494000	-0.452410000
H	-0.623535000	1.074259000	1.263983000
H	2.808265000	-1.035138000	0.245576000
H	0.534333000	-1.248737000	0.936772000

### **1b (M06-2X/cc-pVTZ)**

S	-2.103229000	-0.068262000	-0.163713000
C	-0.467625000	0.642048000	0.310797000
C	0.675464000	-0.311373000	0.430148000
S	2.121265000	0.047602000	-0.217644000
H	-1.744632000	-0.846914000	-1.213518000
H	-2.199216000	-1.089238000	0.723491000
H	-0.293949000	1.453816000	-0.397799000
H	-0.654710000	1.087703000	1.297832000
H	2.802758000	-1.036732000	0.232419000
H	0.554156000	-1.222127000	1.013615000

### **2a (M06-2X/cc-pVTZ)**

S	-2.180273000	-0.153797000	0.002981000
C	0.477081000	-0.422862000	0.017367000
S	2.220649000	0.016181000	-0.105318000
H	-2.662791000	0.576646000	-1.035640000
H	-2.710507000	0.649316000	0.960638000
H	-0.373547000	1.552288000	0.022474000
H	2.195918000	1.241941000	0.473523000
C	-0.491025000	0.475316000	0.019263000
H	0.329593000	-1.498518000	-0.007618000
H	2.658992000	-0.634533000	1.004234000

**2b (M06-2X/cc-pVTZ)**

S	-2.223396000	-0.011058000	-0.102973000
C	-0.485730000	0.445881000	0.036409000
C	0.485730000	-0.445875000	0.036406000
S	2.223397000	0.011053000	-0.102972000
H	-2.166962000	-1.291079000	0.339085000
H	-0.358771000	1.523129000	0.014430000
H	0.358768000	-1.523124000	0.014424000
H	2.166966000	1.291088000	0.339049000
H	-2.660494000	0.505604000	1.075610000
H	2.660482000	-0.505577000	1.075630000

**3 (M06-2X /cc-pVTZ)**

S	1.678821000	-0.482509000	-0.000001000
C	-0.661132000	1.006449000	-0.000001000
S	-1.678821000	-0.482509000	0.000000000
H	2.528091000	-0.131906000	1.001096000
H	2.528109000	-0.131896000	-1.001078000
H	1.206053000	1.945250000	0.000005000
H	-2.528099000	-0.131904000	1.001089000
C	0.661132000	1.006449000	-0.000002000
H	-1.206053000	1.945250000	0.000010000
H	-2.528101000	-0.131899000	-1.001086000

**4 (M06-2X /cc-pVTZ)**

C	2.303173000	0.450069000	-0.319007000
S	1.112054000	-0.545079000	0.122912000
C	-0.303148000	0.572766000	0.484323000
S	-1.862122000	-0.070745000	-0.279188000
H	3.262219000	-0.022226000	-0.538436000
H	2.212384000	1.531665000	-0.393347000
H	-0.418796000	0.637648000	1.566139000
H	-2.666501000	0.943341000	0.133757000
H	-2.251699000	-0.929006000	0.697531000
H	-0.136667000	1.554742000	0.042874000

**5 (M06-2X /cc-pVTZ)**

C	-0.841880000	1.182101000	-0.185275000
C	0.064845000	0.304042000	0.573721000
S	-1.390250000	-0.577188000	-0.143296000
S	1.661212000	-0.163361000	-0.182587000
H	-1.471456000	1.867618000	0.373339000
H	-0.601236000	1.473139000	-1.204273000
H	0.078780000	0.348979000	1.657626000
H	-2.135763000	-0.533006000	0.988789000
H	2.061097000	-1.083912000	0.733529000
H	2.395382000	0.859106000	0.334453000

**6 (M06-2X /cc-pVTZ)**

S	-1.372388000	0.000002000	0.014442000
C	0.000025000	1.223147000	-0.164850000
C	0.000020000	-1.223142000	-0.164887000
S	1.372383000	-0.000002000	0.014819000
H	-1.456988000	-0.000024000	1.369618000
H	0.000172000	1.608367000	-1.185851000
H	-0.000076000	2.025717000	0.571208000
H	1.456630000	-0.000016000	1.370019000
H	-0.000085000	-2.025734000	0.571148000
H	0.000158000	-1.608331000	-1.185900000

**7 (M06-2X/cc-pVTZ)**

C	-2.471087000	0.392334000	0.002914000
S	-0.927290000	-0.541539000	-0.002468000
C	0.258584000	0.539981000	-0.001615000
S	1.963657000	-0.094944000	-0.003085000
H	-2.289528000	1.463404000	-0.017063000
H	-3.014991000	0.039056000	-0.878510000
H	-2.992650000	0.068681000	0.909077000
H	0.120340000	1.620232000	-0.001307000
H	2.449328000	0.737625000	-0.966849000
H	2.420647000	0.660838000	1.035709000



**8 (M06-2X/cc-pVTZ)**

C	2.266692000	0.615121000	0.309280000
S	0.966038000	-0.577937000	-0.218354000
C	-0.501927000	0.402409000	-0.392985000
S	-1.950210000	-0.017112000	0.206992000
H	1.936199000	1.156528000	1.190782000
H	3.125625000	-0.030741000	0.505191000
H	2.452340000	1.246762000	-0.559110000
H	0.666963000	-1.235458000	0.930995000
H	-0.364759000	1.275474000	-1.032879000
H	-2.658203000	1.003045000	-0.350950000

**9 (M06-2X/cc-pVTZ)**

C	-2.076399000	-0.534031000	0.396591000
S	-0.793455000	0.650341000	-0.143673000
S	0.975435000	-0.579810000	-0.254353000
C	2.086343000	0.371296000	0.440871000
H	-1.897104000	-0.718380000	1.454700000
H	-3.004009000	0.030957000	0.256165000
H	-2.056011000	-1.431182000	-0.217752000
H	-1.009348000	0.646891000	-1.486679000
H	1.901452000	1.373620000	0.828883000
H	3.093686000	-0.053992000	0.508336000

**10 (M06-2X/cc-pVTZ)**

C	1.489130000	-0.468459000	0.727484000
C	1.489113000	-0.468508000	-0.727463000
S	0.281433000	0.795481000	-0.000021000
S	-1.535592000	-0.340834000	0.000015000
H	2.246402000	0.094697000	1.269795000
H	0.999486000	-1.265517000	1.279043000
H	2.246367000	0.094615000	-1.269833000
H	0.999457000	-1.265603000	-1.278958000
H	-2.147305000	0.344574000	-1.008244000
H	-2.147326000	0.344688000	1.008182000

**11 (M06-2X/cc-pVTZ)**

C	0.743051000	1.221090000	0.188250000
C	-0.743052000	1.221089000	-0.188250000
S	1.075375000	-0.615251000	0.012614000
S	-1.075375000	-0.615252000	-0.012614000
H	0.940941000	1.433671000	1.239456000
H	1.407189000	1.797525000	-0.454671000
H	-1.407193000	1.797522000	0.454671000
H	-0.940942000	1.433670000	-1.239456000
H	-1.178005000	-0.713715000	1.343592000
H	1.178005000	-0.713713000	-1.343592000

**12 (M06-2X/cc-pVTZ)**

S	1.297209000	-0.526131000	-0.068757000
S	-0.578626000	0.332359000	-0.578458000
C	0.607114000	1.041841000	0.574749000
H	0.843939000	-1.342782000	0.921874000
C	-1.854958000	-0.489381000	0.414307000
H	0.338136000	1.052829000	1.628737000
H	1.136123000	1.907526000	0.176907000
H	-1.519303000	-0.662349000	1.435517000
H	-2.682369000	0.231382000	0.379217000
H	-2.126775000	-1.401001000	-0.121151000

**13 (M06-2X/cc-pVTZ)**

C	2.222900000	-0.333069000	0.000001000
S	0.714807000	0.632281000	-0.000001000
S	-0.714807000	-0.632281000	-0.000001000
C	-2.222901000	0.333069000	0.000001000
H	2.038281000	-1.405963000	0.000001000
H	2.764862000	0.013868000	-0.893302000
H	2.764860000	0.013868000	0.893306000
H	-2.038281000	1.405963000	-0.000010000
H	-2.764867000	-0.013877000	-0.893296000
H	-2.764855000	-0.013860000	0.893312000

**14 (M06-2X/cc-pVTZ)**

S	0.654529000	1.060660000	-0.151347000
S	0.654548000	-1.060654000	-0.151345000
C	-0.693155000	0.000004000	0.560511000
C	-1.990535000	-0.000013000	-0.182159000
H	1.410628000	1.240026000	0.968944000
H	1.410630000	-1.240005000	0.968958000
H	-0.686962000	0.000000000	1.649341000
H	-2.553546000	0.885210000	0.126099000
H	-2.553464000	-0.885331000	0.125972000
H	-1.870375000	0.000071000	-1.266361000