

Dynamic and Static Behavior of the E–E' Bonds (E, E' = S and Se) in Cystine and Derivatives, Elucidated by AIM Dual Functional Analysis

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Optimized structures given by Cartesian coordinates for **1–6**, together with the total energies and the first frequency of the internal vibrations with the 6-311+G(3d) basis sets for S and Se and the 6-311++G(d,p) basis sets for O, N, C and H at the M062X level of the Gaussian 09 program.

1a (C₁): M062X/6-311+G(3d) for S and 6-311++G(d, p) for C, N, O and H.

$E = -1442.629316$ au, $\nu = 511.2703$ cm⁻¹

1	16	0	1.363932	1.695491	0.706082
2	16	0	0.097604	2.387514	-0.767498
3	6	0	-0.953468	0.954782	-1.118905
4	6	0	2.394665	0.447434	-0.147433
5	6	0	-2.075942	0.631709	-0.110828
6	6	0	2.278612	-0.971452	0.466732
7	6	0	-2.443201	-0.857213	-0.218124
8	8	0	-2.148369	-1.545520	-1.164909
9	8	0	-3.145189	-1.313911	0.802338
10	7	0	-1.897744	0.945309	1.299747
11	1	0	-2.977466	1.166179	-0.432784
12	1	0	-3.105648	-0.622289	1.492118
13	1	0	-1.005945	0.588568	1.635816
14	1	0	-1.914377	1.946549	1.451631
15	1	0	-1.396444	1.179791	-2.092768
16	1	0	-0.304482	0.099277	-1.289112
17	1	0	2.439454	-0.903340	1.544398
18	1	0	3.435726	0.768887	-0.071296
19	1	0	2.119000	0.435963	-1.204445
20	7	0	3.219455	-1.925250	-0.093788
21	6	0	0.858207	-1.472668	0.288115
22	8	0	-0.021751	-1.295238	1.091668
23	8	0	0.665257	-2.047943	-0.899341
24	1	0	3.036934	-2.081074	-1.079496
25	1	0	4.173446	-1.600902	0.013074
26	1	0	-0.289573	-2.220760	-1.021585

1b (C_1): M062X/6-311+G(3d) for S and 6-311++G(d, p) for C, N, O and H. $E = -1442.6291965$ au, $\nu = 522.5384$ cm^{-1}

1	16	0	0.410381	1.942814	-0.634161
2	16	0	-0.900663	2.028903	0.935709
3	6	0	-1.708834	0.391261	1.002538
4	6	0	1.918495	1.131454	-0.017770
5	6	0	-2.055994	-0.180595	-0.366824
6	6	0	1.915599	-0.397456	-0.204909
7	6	0	-2.515051	-1.627583	-0.156462
8	8	0	-1.744793	-2.515704	0.086332
9	8	0	-3.830327	-1.807418	-0.235621
10	7	0	-3.110479	0.600265	-1.010354
11	1	0	-1.134940	-0.233677	-0.954737
12	1	0	-4.206840	-0.940180	-0.485016
13	1	0	-3.011551	0.592539	-2.019577
14	1	0	-3.062137	1.570742	-0.714866
15	1	0	-1.051641	-0.295148	1.527570
16	1	0	-2.621077	0.569548	1.582523
17	1	0	1.599968	-0.610873	-1.229982
18	1	0	2.042905	1.384449	1.036743
19	1	0	2.727637	1.589601	-0.592630
20	7	0	1.025899	-1.037535	0.738105
21	6	0	3.354534	-0.885744	-0.067272
22	8	0	3.784699	-1.499710	0.867767
23	8	0	4.112926	-0.513130	-1.113528
24	1	0	0.560891	-1.852625	0.350000
25	1	0	1.546622	-1.336493	1.557734
26	1	0	5.014210	-0.824789	-0.952196

1c (C_1): M062X/6-311+G(3d) for S and 6-311++G(d, p) for C, N, O and H. $E = -1442.6290467$ au, $\nu = 506.8351$ cm^{-1}

1	16	0	-0.622652	1.784461	-1.006404
2	16	0	0.419155	1.923396	0.756981
3	6	0	1.406191	0.402299	0.907313
4	6	0	-2.150572	0.932225	-0.519915
5	6	0	2.455139	0.168941	-0.175901
6	6	0	-1.937841	-0.464263	0.076047
7	6	0	3.493922	-0.841235	0.364981
8	8	0	3.958290	-0.759536	1.467501
9	8	0	3.827398	-1.783170	-0.506879
10	7	0	1.923345	-0.316785	-1.450429
11	1	0	3.012774	1.096822	-0.336124
12	1	0	3.264150	-1.610386	-1.294381
13	1	0	0.969000	-0.658998	-1.329480
14	1	0	1.878822	0.425355	-2.136707
15	1	0	1.913110	0.534246	1.867097
16	1	0	0.754601	-0.469677	0.985148
17	1	0	-1.441994	-0.336781	1.044557
18	1	0	-2.728434	0.864668	-1.449143
19	1	0	-2.703714	1.552479	0.184381
20	7	0	-1.120767	-1.304547	-0.780466
21	6	0	-3.309013	-1.070456	0.361643
22	8	0	-3.757480	-2.037811	-0.185746
23	8	0	-3.970390	-0.380934	1.305024
24	1	0	-1.092045	-2.247596	-0.402499
25	1	0	-1.568341	-1.395352	-1.689876
26	1	0	-4.829519	-0.804628	1.439848

2a (C_1): M062X/6-311+G(3d) for S and Se and 6-311++G(d, p) for C, N, O and H. $E = -3446.0085859$ au, $\nu = 414.4146$ cm^{-1}

1	16	0	0.077689	-1.921698	1.013398
2	34	0	-1.406730	-1.307631	-0.487351
3	6	0	-2.551025	-0.078146	0.556856
4	6	0	1.338800	-0.605188	1.006331
5	6	0	-2.404232	1.382615	0.122123
6	6	0	1.938995	-0.320501	-0.371016
7	6	0	-1.009289	1.860797	0.525114
8	8	0	-0.644120	1.885252	1.673538
9	8	0	-0.239486	2.184767	-0.508588
10	7	0	-2.768893	1.535012	-1.273835
11	1	0	-3.106385	1.958760	0.733743
12	1	0	0.685518	2.342286	-0.209106
13	1	0	-2.013115	1.195174	-1.861872
14	1	0	-2.886676	2.514875	-1.505082
15	1	0	-3.575257	-0.403557	0.379726
16	1	0	-2.281909	-0.218615	1.602554
17	1	0	1.130869	-0.012142	-1.042368
18	1	0	2.116066	-0.987538	1.678165
19	1	0	0.926321	0.302913	1.443695
20	7	0	2.700770	-1.466039	-0.862611
21	6	0	2.867610	0.888560	-0.211869
22	8	0	2.450372	2.010035	-0.054062
23	8	0	4.157209	0.605314	-0.224779
24	1	0	2.656992	-1.531520	-1.873702
25	1	0	2.314814	-2.330468	-0.494178
26	1	0	4.218472	-0.358132	-0.394979

2b (C_1): M062X/6-311+G(3d) for S and Se and 6-311++G(d, p) for C, N, O and H. $E = -3446.0026241$ au, $\nu = 423.5810$ cm^{-1}

1	16	0	-1.875670	-1.702064	0.502745
2	34	0	-0.133458	-1.220709	-0.732024
3	6	0	1.344298	-1.259398	0.579574
4	6	0	-2.416830	-0.122677	1.252144
5	6	0	2.614597	-0.598805	0.011327
6	6	0	-2.395275	1.129560	0.371333
7	6	0	2.278458	0.862455	-0.262880
8	8	0	2.286703	1.706931	0.603018
9	8	0	1.908414	1.094174	-1.514898
10	7	0	3.684136	-0.777423	0.975207
11	1	0	2.890547	-1.080019	-0.930139
12	1	0	1.412165	1.932180	-1.542862
13	1	0	4.573483	-0.484408	0.585516
14	1	0	3.507642	-0.195557	1.789323
15	1	0	1.012799	-0.721342	1.469693
16	1	0	1.570780	-2.293302	0.829620
17	1	0	-2.938145	1.888436	0.953946
18	1	0	-1.851217	0.055870	2.163931
19	1	0	-3.455601	-0.336992	1.515890
20	7	0	-3.094922	0.937894	-0.876175
21	6	0	-0.999031	1.742580	0.236550
22	8	0	-0.576068	2.272099	-0.761575
23	8	0	-0.334988	1.720834	1.395141
24	1	0	-2.950530	1.739985	-1.480392
25	1	0	-2.727785	0.127511	-1.364751
26	1	0	0.549851	2.106883	1.260116

2c (C_1): M062X/6-311+G(3d) for S and Se and 6-311++G(d, p) for C, N, O and H. $E = -3446.0019381$ au, $\nu = 414.7042$ cm^{-1}

1	16	0	-0.845057	-1.746305	0.884283
2	34	0	0.334495	-1.213319	-0.895960
3	6	0	2.136125	-1.118611	-0.085791
4	6	0	-1.462291	-0.178086	1.573075
5	6	0	2.814937	0.248421	-0.218952
6	6	0	-2.579915	0.502854	0.763731
7	6	0	1.831845	1.301934	0.275776
8	8	0	1.464177	1.349147	1.423708
9	8	0	1.413129	2.110802	-0.687653
10	7	0	4.049825	0.197407	0.551428
11	1	0	3.054453	0.454071	-1.263590
12	1	0	0.603778	2.568939	-0.388171
13	1	0	4.619871	1.016874	0.372049
14	1	0	3.824208	0.196106	1.542707
15	1	0	1.985424	-1.349878	0.969388
16	1	0	2.758724	-1.886464	-0.541451
17	1	0	-3.093686	1.182121	1.451298
18	1	0	-0.636140	0.514020	1.742327
19	1	0	-1.860688	-0.489816	2.543217
20	7	0	-3.551697	-0.396491	0.148843
21	6	0	-1.992779	1.446891	-0.299612
22	8	0	-1.196800	2.304770	-0.012900
23	8	0	-2.470234	1.279325	-1.518042
24	1	0	-4.442108	-0.395803	0.627690
25	1	0	-3.196545	-1.348008	0.111073
26	1	0	-3.125826	0.552362	-1.444595

3a (C_1): M062X/6-311+G(3d) for Se and 6-311++G(d, p) for C, N, O and H. $E = -5449.3744678$ au, $\nu = 301.9359$ cm^{-1}

1	34	0	-0.221890	-0.949864	-1.289465
2	34	0	-1.423724	-1.470442	0.634531
3	6	0	-1.805643	0.227218	1.580206
4	6	0	1.638208	-0.982265	-0.649037
5	6	0	-2.303671	1.413553	0.754190
6	6	0	2.038039	0.308142	0.079900
7	6	0	-1.151319	2.092627	0.009552
8	8	0	-1.164635	2.377180	-1.157662
9	8	0	-0.131519	2.357704	0.832257
10	7	0	-3.438101	1.065617	-0.068534
11	1	0	-2.629282	2.156522	1.495300
12	1	0	0.676252	2.529770	0.293038
13	1	0	-3.189462	0.312648	-0.703230
14	1	0	-3.697572	1.856873	-0.648284
15	1	0	-2.605316	-0.093296	2.251644
16	1	0	-0.933278	0.507431	2.163646
17	1	0	1.412608	0.386788	0.976826
18	1	0	2.242257	-1.116015	-1.551573
19	1	0	1.752758	-1.851066	-0.002590
20	7	0	1.929087	1.525908	-0.714707
21	6	0	3.473865	0.155340	0.547951
22	8	0	4.416438	0.723300	0.070941
23	8	0	3.574822	-0.732757	1.547074
24	1	0	2.830620	1.764503	-1.117544
25	1	0	1.246539	1.421034	-1.462204
26	1	0	4.510122	-0.816580	1.777949

3b (C_1): M062X/6-311+G(3d) for Se and 6-311++G(d, p) for C, N, O and H. $E = -5449.373934$ au, $\nu = 308.0088$ cm^{-1}

1	34	0	-0.921922	-1.653792	0.548847
2	34	0	0.480949	-0.903805	-1.154050
3	6	0	2.235228	-1.040778	-0.246524
4	6	0	-1.492389	-0.008089	1.470660
5	6	0	2.981359	0.292570	-0.138839
6	6	0	-2.511105	0.853740	0.712270
7	6	0	2.016677	1.316719	0.446257
8	8	0	1.581038	1.223516	1.567447
9	8	0	1.696425	2.271715	-0.415378
10	7	0	4.162553	0.066583	0.682417
11	1	0	3.294533	0.631917	-1.127557
12	1	0	0.885558	2.721698	-0.106874
13	1	0	3.877911	-0.060222	1.650028
14	1	0	4.781667	0.869275	0.651365
15	1	0	2.022252	-1.422002	0.752379
16	1	0	2.843526	-1.762273	-0.788812
17	1	0	-2.968630	1.519311	1.451781
18	1	0	-0.611333	0.575698	1.737098
19	1	0	-1.949103	-0.400140	2.382854
20	7	0	-3.562623	0.132718	0.000613
21	6	0	-1.798872	1.821930	-0.248057
22	8	0	-0.924995	2.559157	0.131914
23	8	0	-2.254722	1.817359	-1.485687
24	1	0	-3.303830	-0.837273	-0.157775
25	1	0	-4.451589	0.163789	0.481118
26	1	0	-2.994768	1.172887	-1.490915

3c (C_1): M062X/6-311+G(3d) for Se and 6-311++G(d, p) for C, N, O and H. $E = -5449.3732093$ au, $\nu = 298.6601$ cm^{-1}

1	34	0	0.348849	-0.889881	-0.928490
2	34	0	-1.549536	-1.475135	0.290809
3	6	0	-1.906565	0.142971	1.354755
4	6	0	1.756864	-1.499767	0.315673
5	6	0	-2.415360	1.344359	0.551845
6	6	0	2.514586	-0.353022	0.965297
7	6	0	-1.254675	2.094813	-0.131893
8	8	0	-0.253222	2.399555	0.459528
9	8	0	-1.480568	2.427154	-1.391881
10	7	0	-3.469038	1.063685	-0.419938
11	1	0	-2.796879	2.073292	1.275414
12	1	0	-2.375450	2.086798	-1.600354
13	1	0	-4.392536	1.254728	-0.054675
14	1	0	-3.431880	0.094763	-0.726887
15	1	0	-2.678447	-0.185196	2.055226
16	1	0	-1.006101	0.394283	1.914474
17	1	0	3.281239	-0.792558	1.616010
18	1	0	2.424547	-2.123886	-0.276590
19	1	0	1.260572	-2.095760	1.078101
20	7	0	1.646618	0.466842	1.796623
21	6	0	3.270770	0.436242	-0.101578
22	8	0	3.296168	0.173085	-1.273443
23	8	0	3.924217	1.485155	0.424116
24	1	0	1.060206	1.068597	1.219623
25	1	0	2.204161	1.084819	2.376168
26	1	0	4.344370	1.963803	-0.303312

4 (C_2): M062X/6-311+G(3d) for S and 6-311++G(d, p) for C and H.

$E = -876.1780226$ au, $\nu = 513.7069$ cm^{-1}

1	1	0	-0.268681	2.360564	0.567134
2	1	0	-1.987697	1.976908	0.839386
3	1	0	-0.738540	1.123144	1.771252
4	6	0	-0.975900	1.568678	0.806193
5	16	0	-0.975900	0.312015	-0.500933
6	16	0	0.975900	-0.312015	-0.500933
7	6	0	0.975900	-1.568678	0.806193
8	1	0	0.268681	-2.360564	0.567134
9	1	0	1.987697	-1.976908	0.839386
10	1	0	0.738540	-1.123144	1.771252

5 (C_1): M062X/6-311+G(3d) for S and Se and 6-311++G(d, p) for C and H.

$E = -2879.5481642$ au, $\nu = 419.7233$ cm^{-1}

1	1	0	-2.148588	-0.029279	-1.563347
2	1	0	-3.184576	0.690641	-0.306100
3	1	0	-1.748779	1.571709	-0.872671
4	6	0	-2.158880	0.584685	-0.664883
5	16	0	-1.239734	-0.227720	0.671789
6	34	0	0.763085	-0.437699	-0.194718
7	6	0	1.498186	1.318143	0.263994
8	1	0	1.454188	1.455744	1.341276
9	1	0	2.535741	1.317693	-0.071451
10	1	0	0.947044	2.101825	-0.250577

6 (C_2): M062X/6-311+G(3d) for Se and 6-311++G(d, p) for C and H.

$E = -4882.9205598$ au, $\nu = 307.6595$ cm^{-1}

1	1	0	1.569891	1.926018	0.829660
2	1	0	0.143184	2.945255	1.161478
3	1	0	0.360602	1.415840	2.047846
4	6	0	0.516762	1.922679	1.098734
5	34	0	-0.516762	1.040553	-0.312688
6	34	0	0.516762	-1.040553	-0.312688
7	6	0	-0.516762	-1.922679	1.098734
8	1	0	-1.569891	-1.926018	0.829660
9	1	0	-0.143184	-2.945255	1.161478
10	1	0	-0.360602	-1.415840	2.047846