Supplementary data for article:

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Unusual Mode of Reactivity of 2-Alkylidene-4-oxothiazolidine *S*-oxides Under the Pummerer Reaction Conditions

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Supplementary Data

Table of Contents:

Absolute energies (atomic units) and x, y, z coordinates (Å) of the optimized structures

10a-*Z*

E = -1449.7236962 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.501021	0.521322	-0.237553
2	1	0	-4.275513	0.745708	0.498383
3	1	0	-3.936670	0.586214	-1.238564
4	7	0	-1.600782	-0.925575	0.132668
5	6	0	-0.994140	-2.167953	0.628998
6	1	0	-0.288050	-1.923535	1.426009
7	1	0	-1.807088	-2.780164	1.018571
8	1	0	-0.467560	-2.692484	-0.166153
9	6	0	-2.988860	-0.886674	0.003012
10	6	0	-0.936699	0.290620	0.018207
11	6	0	0.411548	0.519009	0.007390
12	6	0	1.467910	-0.466802	-0.291287
13	16	0	-2.079953	1.654298	-0.078332
14	17	0	0.929032	2.197913	0.156211
15	8	0	-3.709976	-1.861834	0.096886
16	8	0	1.276417	-1.510120	-0.900082
17	8	0	2.682388	-0.074623	0.135910
18	6	0	3.795667	-0.933934	-0.218105
19	1	0	3.631279	-1.919244	0.228931
20	1	0	3.807909	-1.056791	-1.305319
21	6	0	5.059797	-0.275323	0.299598
22	1	0	5.924817	-0.899760	0.052824
23	1	0	5.203872	0.709207	-0.154986
24	1	0	5.022332	-0.152385	1.386086

10a-*E*

E = -1449.7258336 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.973982	-1.585346	-0.152190
2	1	0	3.513580	-2.100860	0.645925
3	1	0	3.342591	-1.953937	-1.113821
4	7	0	2.063769	0.637293	0.045707
5	6	0	2.206122	2.079882	0.302100
6	1	0	1.621126	2.364780	1.175855
7	1	0	3.266100	2.249271	0.488271
8	1	0	1.890624	2.667360	-0.559592
9	6	0	3.244511	-0.104747	-0.048279
10	8	0	4.357582	0.389321	-0.035416
11	16	0	1.170952	-1.841735	-0.004427
12	6	0	0.867938	-0.080142	0.018008
13	6	0	-0.413067	0.412293	-0.007881
14	17	0	-0.804048	2.120772	-0.173604
15	6	0	-1.557778	-0.508122	0.046632
16	8	0	-1.429199	-1.724959	0.135039
17	8	0	-2.753760	0.101299	-0.006153
18	6	0	-3.914911	-0.766157	0.049805
19	1	0	-3.868791	-1.350423	0.973779
20	1	0	-3.868464	-1.463980	-0.791660
21	6	0	-5.144532	0.119589	-0.007899
22	1	0	-6.044933	-0.502292	0.032695
23	1	0	-5.167450	0.815091	0.836259
24	1	0	-5.167763	0.699792	-0.935105

10b-*Z*

E = -1526.9174146 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.058714	0.426002	0.148081
2	1	0	-4.651355	0.654310	1.036491
3	1	0	-4.713423	0.449877	-0.727113
4	7	0	-2.078293	-0.957792	0.157244
5	6	0	-1.347631	-2.191407	0.461574
6	1	0	-0.533280	-1.966052	1.155233
7	1	0	-2.059856	-2.872711	0.925712
8	1	0	-0.931614	-2.631564	-0.444831
9	6	0	-3.464700	-0.962728	0.296195
10	6	0	-1.481732	0.275441	-0.086420
11	8	0	-4.125015	-1.957749	0.529807
12	16	0	-2.674189	1.597488	-0.049048
13	6	0	-0.155539	0.530637	-0.288531
14	17	0	0.318491	2.235572	-0.364353
15	6	0	0.895007	-0.441624	-0.693697
16	8	0	0.606217	-1.364804	-1.455965
17	6	0	2.294868	-0.287915	-0.189959
18	6	0	3.338353	-0.841959	-0.949371
19	6	0	2.585532	0.310783	1.046253
20	6	0	4.652073	-0.782487	-0.488558
21	1	0	3.099552	-1.315281	-1.896057
22	6	0	3.899180	0.352746	1.514774
23	1	0	1.785586	0.732556	1.646084
24	6	0	4.934522	-0.186278	0.745498
25	1	0	5.455271	-1.202066	-1.087054
26	1	0	4.114896	0.807743	2.476900
27	1	0	5.958002	-0.143672	1.106945

10b-*E*

E = -1526.9161601 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.661618	-1.451993	-0.176400
2	1	0	4.178321	-1.920455	0.665717
3	1	0	4.121800	-1.805468	-1.103014
4	7	0	2.580836	0.693361	-0.000743
5	16	0	1.873169	-1.841294	-0.123177
6	6	0	3.818055	0.045311	-0.097190
7	8	0	4.883948	0.631724	-0.142334
8	6	0	2.588889	2.158091	-0.146945
9	1	0	2.346310	2.652607	0.793116
10	1	0	3.601431	2.427226	-0.445814
11	1	0	1.877128	2.459273	-0.915179
12	6	0	1.450150	-0.118622	0.030647
13	6	0	0.134760	0.269269	0.174741
14	6	0	-0.947636	-0.715436	0.043791
15	8	0	-0.658760	-1.918571	-0.010228
16	17	0	-0.310961	1.890681	0.724095
17	6	0	-2.391283	-0.318689	-0.042049
18	6	0	-2.845865	0.738046	-0.845502
19	6	0	-3.326832	-1.125929	0.623990
20	6	0	-4.213431	0.986576	-0.971572
21	1	0	-2.137210	1.355625	-1.386772
22	6	0	-4.691387	-0.858589	0.518960
23	1	0	-2.970982	-1.961200	1.218283
24	6	0	-5.137898	0.197499	-0.281240
25	1	0	-4.556429	1.797263	-1.607704
26	1	0	-5.405865	-1.478701	1.052314
27	1	0	-6.201070	0.401004	-0.371422

10c-*Z*

E = -1582.2947292 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.533087	-0.003250	-0.280468
2	1	0	-5.352334	0.140067	0.426581
3	1	0	-4.949444	-0.114746	-1.285508
4	7	0	-2.405468	-1.028801	0.233114
5	16	0	-3.351651	1.385176	-0.222519
6	6	0	-3.772501	-1.261690	0.096715
7	6	0	-1.974435	0.273685	0.004994
8	6	0	-0.691212	0.737969	-0.029058
9	6	0	0.546360	-0.065682	-0.231674
10	6	0	-1.585158	-2.088807	0.834099
11	1	0	-0.963094	-2.573893	0.084082
12	1	0	-0.942536	-1.649013	1.600238
13	1	0	-2.274706	-2.803211	1.283163
14	8	0	-4.303181	-2.340762	0.281142
15	17	0	-0.500326	2.504704	-0.048163
16	8	0	0.505735	-1.158694	-0.799629
17	7	0	1.703224	0.509140	0.233228
18	6	0	3.035624	0.062800	0.096544
19	6	0	4.038518	0.893346	0.627649
20	6	0	3.395767	-1.143023	-0.526985
21	6	0	5.379578	0.528796	0.537362
22	1	0	3.763708	1.828027	1.111463
23	6	0	4.746107	-1.492288	-0.611197
24	1	0	2.628752	-1.784913	-0.935522
25	6	0	5.743640	-0.669217	-0.085005
26	1	0	6.139434	1.183882	0.953288
27	1	0	5.014547	-2.425748	-1.097592
28	1	0	6.788442	-0.955010	-0.157158
29	1	0	1.599270	1.409220	0.681679

10c-*E*

E = -1582.2967078 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.735529	-1.853258	-0.204363
2	1	0	4.204871	-2.471023	0.564926
3	1	0	4.038917	-2.231545	-1.185108
4	7	0	3.148145	0.466724	0.068710
5	16	0	1.912859	-1.859919	-0.039633
6	6	0	4.213207	-0.431866	-0.047544
7	6	0	1.862607	-0.074701	0.015056
8	6	0	0.666703	0.595106	-0.013956
9	6	0	-0.615013	-0.146628	0.029029
10	8	0	5.383948	-0.097916	-0.011017
11	8	0	-0.601361	-1.380627	0.120584
12	6	0	3.491334	1.856117	0.410662
13	1	0	3.309883	2.529806	-0.426802
14	1	0	2.917379	2.180854	1.278311
15	1	0	4.555332	1.855353	0.645101
16	17	0	0.563596	2.359537	-0.189613
17	7	0	-1.767985	0.590954	-0.032475
18	6	0	-3.107139	0.144608	-0.002200
19	6	0	-4.103125	1.135987	-0.057759
20	6	0	-3.481893	-1.206524	0.075688
21	6	0	-5.451130	0.786857	-0.036879
22	1	0	-3.817244	2.183867	-0.117457
23	6	0	-4.838862	-1.539366	0.096140
24	1	0	-2.720882	-1.972048	0.118333
25	6	0	-5.829392	-0.557004	0.040401
26	1	0	-6.204958	1.567467	-0.080885
27	1	0	-5.118009	-2.587461	0.156378
28	1	0	-6.879499	-0.831898	0.056896
29	1	0	-1.651436	1.591844	-0.108006

10d-*Z*

E = -1660.9289774 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.274229	-0.317926	-0.702785
2	1	0	-6.217037	-0.212401	-0.162860
3	1	0	-5.490903	-0.524584	-1.754576
4	7	0	-3.199159	-1.111691	0.248163
5	16	0	-4.241056	1.175894	-0.537033
6	6	0	-4.494752	-1.476872	-0.107656
7	6	0	-2.839841	0.211165	0.005837
8	6	0	-1.614786	0.788437	0.163611
9	6	0	-0.295045	0.102076	0.259349
10	17	0	-1.563774	2.560794	0.044250
11	8	0	-4.962577	-2.588104	0.058521
12	8	0	-0.125566	-1.025802	-0.215144
13	6	0	-2.417546	-2.054847	1.059081
14	1	0	-1.625629	-2.512794	0.469442
15	1	0	-1.970723	-1.515380	1.897421
16	1	0	-3.115053	-2.808962	1.422928
17	7	0	0.709027	0.788440	0.877085
18	1	0	0.530047	1.734832	1.179968
19	6	0	2.080571	0.293801	0.898308
20	1	0	2.042022	-0.793391	0.995951
21	1	0	2.569063	0.695153	1.791895
22	6	0	2.884520	0.675174	-0.365357
23	1	0	2.901678	1.767389	-0.461753
24	1	0	2.354448	0.279425	-1.238071
25	6	0	4.297967	0.136444	-0.321616
26	6	0	4.573364	-1.179751	-0.723859
27	6	0	5.357650	0.923850	0.152202
28	6	0	5.870209	-1.694072	-0.654599
29	1	0	3.765145	-1.802613	-1.100058
30	6	0	6.656973	0.413832	0.223063
31	1	0	5.165723	1.949391	0.460253
32	6	0	6.917177	-0.898406	-0.179999
33	1	0	6.063663	-2.713826	-0.975542
34	1	0	7.464621	1.042594	0.587440
35	1	0	7.926661	-1.296058	-0.129397

10d-*E*

E = -1660.931233 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.126812	-2.215019	-0.320943
2	1	0	4.573158	-2.910471	0.393596
3	1	0	4.214002	-2.645309	-1.323235
4	7	0	4.032649	0.176132	-0.054797
5	16	0	2.376251	-1.871700	0.091845
6	6	0	4.883014	-0.911024	-0.270753
7	6	0	2.671080	-0.108289	0.072200
8	6	0	1.630489	0.776848	0.158335
9	6	0	0.247157	0.301580	0.389851
10	17	0	1.830437	2.524415	-0.081083
11	8	0	6.091233	-0.809387	-0.390784
12	8	0	0.031183	-0.909058	0.553116
13	6	0	4.669910	1.477259	0.199556
14	1	0	4.518608	2.165680	-0.631951
15	1	0	4.274082	1.913592	1.116577
16	1	0	5.735291	1.276781	0.309347
17	7	0	-0.757364	1.219234	0.430929
18	1	0	-0.544792	2.186679	0.240353
19	6	0	-2.144331	0.822893	0.640711
20	1	0	-2.664297	1.659226	1.118767
21	1	0	-2.150717	-0.019851	1.336224
22	6	0	-2.867287	0.423073	-0.665326
23	1	0	-2.303999	-0.394046	-1.127859
24	1	0	-2.844426	1.271080	-1.360304
25	6	0	-4.297424	-0.001958	-0.412918
26	6	0	-5.355143	0.911688	-0.530900
27	6	0	-4.592767	-1.316344	-0.018696
28	6	0	-6.671656	0.526785	-0.262583
29	1	0	-5.147449	1.932547	-0.844309
30	6	0	-5.906858	-1.705754	0.250677
31	1	0	-3.785753	-2.039589	0.071753
32	6	0	-6.951515	-0.784512	0.130349
33	1	0	-7.476932	1.248884	-0.365326
34	1	0	-6.115318	-2.729134	0.550031
35	1	0	-7.974111	-1.087300	0.336294

10e-*Z*

E = -1680.786738 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.563145	-1.381185	-0.039725
2	1	0	4.354745	-0.985507	0.599286
3	1	0	3.986339	-2.158385	-0.682758
4	7	0	1.624652	-0.160721	-0.823342
5	6	0	0.998880	1.047481	-1.407117
6	1	0	1.814229	1.531642	-1.949934
7	1	0	0.235490	0.741932	-2.119041
8	6	0	3.016608	-0.257756	-0.898976
9	6	0	0.992054	-1.092009	-0.000201
10	6	0	-0.343970	-1.328344	0.171183
11	6	0	-1.450497	-0.920239	-0.713476
12	16	0	2.175849	-2.038057	0.942469
13	17	0	-0.782629	-2.393259	1.508039
14	8	0	3.720434	0.482107	-1.560872
15	8	0	-1.311633	-0.604387	-1.888494
16	8	0	-2.650021	-0.986587	-0.110480
17	6	0	-3.804932	-0.710014	-0.941178
18	1	0	-3.737266	0.322197	-1.298526
19	1	0	-3.773407	-1.370165	-1.813250
20	6	0	-5.040372	-0.938561	-0.091753
21	1	0	-5.936368	-0.734242	-0.687246
22	1	0	-5.088242	-1.973274	0.259989
23	1	0	-5.046380	-0.276573	0.779221
24	6	0	0.420424	1.993321	-0.370235
25	6	0	1.147354	2.366246	0.769525
26	6	0	-0.838844	2.567432	-0.584125
27	6	0	0.622257	3.285309	1.679043
28	1	0	2.131131	1.940840	0.949044
29	6	0	-1.362692	3.496716	0.319683
30	1	0	-1.411637	2.281888	-1.462273
31	6	0	-0.635138	3.855381	1.456051
32	1	0	1.196883	3.561330	2.558531
33	1	0	-2.340571	3.933550	0.137844
34	1	0	-1.042323	4.572398	2.162913

10e-*E*

E = -1680.7879762 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.176975	-3.118119	-0.564566
2	1	0	-1.851107	-3.285748	-1.407337
3	1	0	-0.968374	-4.080870	-0.087990
4	7	0	-1.057829	-1.102075	0.758782
5	6	0	-1.764141	0.025966	1.437081
6	1	0	-2.550411	-0.454931	2.019241
7	1	0	-1.076164	0.513289	2.118055
8	6	0	-1.856153	-2.200913	0.423626
9	8	0	-2.976115	-2.382680	0.866522
10	16	0	0.372278	-2.311606	-1.102020
11	6	0	0.200418	-1.051711	0.156738
12	6	0	1.250126	-0.220400	0.459191
13	17	0	1.296373	0.811180	1.883989
14	6	0	2.461476	-0.224703	-0.373073
15	8	0	2.578373	-0.927083	-1.371380
16	8	0	3.424130	0.609767	0.054933
17	6	0	4.636007	0.645701	-0.741555
18	1	0	4.370781	0.922266	-1.766458
19	1	0	5.065740	-0.360222	-0.765596
20	6	0	5.570715	1.652573	-0.099545
21	1	0	6.500362	1.706680	-0.675662
22	1	0	5.120084	2.649289	-0.078217
23	1	0	5.817115	1.361994	0.925976
24	6	0	-2.363580	1.011979	0.451321
25	6	0	-1.657833	2.157905	0.057224
26	6	0	-3.647149	0.791870	-0.073565
27	6	0	-2.217079	3.058917	-0.852765
28	1	0	-0.670916	2.351280	0.466722
29	6	0	-4.205840	1.692399	-0.983233
30	1	0	-4.206216	-0.086685	0.234866
31	6	0	-3.490996	2.827189	-1.377191
32	1	0	-1.658461	3.942642	-1.147620
33	1	0	-5.201101	1.510472	-1.378690
34	1	0	-3.926388	3.528770	-2.082978

10f-*Z*

E = -1410.4288028 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.579935	0.132455	0.000124
2	1	0	4.209774	0.216156	-0.888523
3	1	0	4.209790	0.216110	0.888750
4	7	0	1.510775	-1.064392	0.000083
5	6	0	2.881655	-1.227047	0.000042
6	6	0	0.996374	0.213004	-0.000190
7	6	0	-0.338019	0.505420	-0.000213
8	6	0	-1.355029	-0.549077	-0.000101
9	16	0	2.280707	1.428792	0.000142
10	17	0	-0.825109	2.187287	-0.000066
11	8	0	3.455640	-2.297416	-0.000154
12	8	0	-1.077419	-1.750741	0.000236
13	8	0	-2.612243	-0.089328	-0.000371
14	6	0	-3.667807	-1.087196	-0.000273
15	1	0	-3.547235	-1.718480	-0.885520
16	1	0	-3.546540	-1.719084	0.884438
17	6	0	-4.990211	-0.345622	0.000466
18	1	0	-5.812918	-1.068162	0.000514
19	1	0	-5.086046	0.286138	0.888369
20	1	0	-5.086697	0.286754	-0.886928
21	1	0	0.850784	-1.844984	0.000356

10f-*E*

E = -1410.4248742 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.263774	-1.185504	0.000069
2	1	0	-3.769652	-1.573967	-0.887478
3	1	0	-3.769553	-1.574069	0.887616
4	7	0	-2.074874	0.877829	-0.000134
5	6	0	-3.347361	0.333355	0.000113
6	8	0	-4.370506	0.988526	0.000326
7	16	0	-1.484614	-1.663489	-0.000109
8	6	0	-0.982101	0.034901	-0.000153
9	6	0	0.308463	0.475914	-0.000119
10	17	0	0.619944	2.206993	-0.000102
11	6	0	1.425223	-0.467503	-0.000021
12	8	0	1.247626	-1.681417	-0.000024
13	8	0	2.635401	0.113121	0.000034
14	6	0	3.775753	-0.785041	0.000060
15	1	0	3.712678	-1.425490	-0.884747
16	1	0	3.712550	-1.425577	0.884794
17	6	0	5.027357	0.070899	0.000197
18	1	0	5.911283	-0.575396	0.000249
19	1	0	5.067106	0.709151	-0.887427
20	1	0	5.066958	0.709086	0.887875
21	1	0	-1.953993	1.884456	-0.000032