

Supporting Information

THE EFFECT OF LITHIUM ION ON THE STEREOSELECTIVITY OF THE INTRAMOLECULAR MICHAEL ADDITION OF AN N-ARYL SULFOXIMINE ANION

**Aswin Garimalla,^{a1} Quin Long,^b Christopher J. Cramer,^b Michael
Harmata***

*^aDepartment of Chemistry, University of Missouri-Columbia, Columbia,
MO 65211*

^bDepartment of Chemistry, University of Minnesota, Minneapolis, MN 55455

harmata@missouri.edu

Cartesian Coordinates (Å) and Electronic Energies (E_h , M06-L/6-31+G(d)/auto) for Lowest
Energy Transition-State Structures.....S2

(R,E)-1⁻ (Figure 1; $E = -1335.874\ 15$)

C	-0.595541	4.338658	-0.023594
C	0.359053	3.378984	0.275410
C	0.053255	2.001317	0.365300
C	-1.302337	1.605289	0.136246
C	-2.240611	2.603176	-0.175163
C	-1.915793	3.953183	-0.259920
H	-0.306642	5.389948	-0.072547
H	1.395936	3.662119	0.455687
C	-1.774279	0.210344	0.253244
H	-3.274222	2.290632	-0.319676
H	-2.684459	4.690498	-0.491040
C	0.016610	-0.787748	-0.683805
H	-1.495205	-0.329807	1.160150
H	-0.266074	-1.838239	-0.685681
H	0.172644	-0.295304	-1.643705
N	1.151468	1.206001	0.656946
S	1.115250	-0.366014	0.522170
O	0.883087	-1.208226	1.720561
C	2.840788	-0.669872	0.077550
C	3.406631	-1.898036	0.426274
C	3.554408	0.238775	-0.706229
C	4.690845	-2.214075	-0.010140
H	2.832591	-2.581283	1.050325
C	4.836862	-0.085484	-1.140893
H	3.097055	1.198395	-0.942381
C	5.409222	-1.311757	-0.796517
H	5.137558	-3.168169	0.271087
H	5.399230	0.627820	-1.744228
H	6.415072	-1.560456	-1.134810
C	-2.929571	-0.226109	-0.379381
C	-3.536733	-1.470882	-0.046817
H	-3.325951	0.306636	-1.242359
O	-3.211120	-2.287163	0.812746
O	-4.652935	-1.715252	-0.857234
C	-5.316105	-2.927092	-0.565982
H	-5.686826	-2.945333	0.467571
H	-6.155493	-2.988613	-1.266202
H	-4.651973	-3.791524	-0.697621

(R,Z)-1⁻ (Figure 2; $E = -1335.869\ 32$)

C	1.275320	3.804600	0.279466
C	0.123773	3.093560	-0.021897
C	0.157398	1.738177	-0.419058
C	1.431139	1.096525	-0.496436
C	2.575918	1.841708	-0.178050
C	2.519979	3.175966	0.206116
H	1.200283	4.852866	0.574139
H	-0.856471	3.567252	0.031309
C	1.579613	-0.270661	-1.023829
H	3.539069	1.342480	-0.255127
H	3.436112	3.717468	0.440940

C	-0.183271	-1.159796	0.141757
H	1.001149	-0.446409	-1.934847
H	-0.130508	-2.230256	-0.041204
H	-0.033199	-0.801528	1.159621
N	-1.093276	1.197168	-0.691593
S	-1.351939	-0.355875	-0.759123
O	-1.502807	-1.022557	-2.079111
C	-3.008593	-0.425043	-0.036744
C	-3.876753	-1.440659	-0.442080
C	-3.369837	0.439911	0.998059
C	-5.109268	-1.587732	0.190247
H	-3.575493	-2.090833	-1.261931
C	-4.601559	0.284579	1.627955
H	-2.682997	1.237852	1.277343
C	-5.475044	-0.728995	1.227992
H	-5.792606	-2.373466	-0.133568
H	-4.887905	0.965404	2.430071
H	-6.440979	-0.844849	1.719520
C	2.675483	-1.114576	-0.883613
C	3.513116	-1.224712	0.266193
H	2.783642	-1.916902	-1.611430
O	3.472545	-0.622570	1.336847
O	4.485209	-2.216086	0.064232
C	5.336807	-2.414363	1.172064
H	4.773335	-2.714776	2.065439
H	6.030586	-3.209831	0.881383
H	5.895042	-1.501883	1.420883

$(R,E)\text{-1}^- \cdot \text{Li}^+$ (Figure 3; $E = -1343.419\ 26$)

C	-0.542320	4.465150	0.074065
C	0.383126	3.480055	0.399732
C	0.037216	2.114117	0.397547
C	-1.299258	1.755823	0.055120
C	-2.211101	2.766681	-0.277624
C	-1.849286	4.112154	-0.274922
H	-0.243044	5.515574	0.093537
H	1.407765	3.737141	0.671832
C	-1.725845	0.344071	0.108871
H	-3.238853	2.481748	-0.510971
H	-2.583876	4.879007	-0.528424
C	-0.058724	-0.501200	-0.963187
H	-1.381469	-0.138729	1.035048
H	-0.297759	-1.541457	-1.215015
H	0.076131	0.191916	-1.798610
N	1.105621	1.249644	0.744032
S	1.019438	-0.289636	0.355631
O	0.616328	-1.378232	1.380104
C	2.745837	-0.671257	0.023128
C	3.183682	-1.980709	0.237612
C	3.599605	0.307054	-0.491939
C	4.498326	-2.319933	-0.081768
H	2.489234	-2.699537	0.669007
C	4.913310	-0.042975	-0.808112

H	3.222243	1.321924	-0.613684
C	5.361235	-1.352281	-0.605681
H	4.854696	-3.337995	0.088946
H	5.594491	0.712235	-1.204555
H	6.391605	-1.617332	-0.850502
C	-2.930718	-0.134184	-0.420824
C	-3.349263	-1.447720	-0.112127
H	-3.494475	0.426560	-1.162562
O	-2.711728	-2.303113	0.582947
O	-4.567841	-1.791314	-0.653759
C	-4.965933	-3.146286	-0.335895
H	-5.075089	-3.282728	0.751948
H	-5.932034	-3.276739	-0.840648
H	-4.229850	-3.875774	-0.710483
Li	-1.014489	-2.106407	1.069503

(*R,Z*)-1⁻ • Li⁺ (Figure 4; *E* = -1343.420 55)

C	1.403296	3.712632	-0.791573
C	0.226146	3.096159	-0.405233
C	0.210067	1.838000	0.234003
C	1.462306	1.213090	0.527261
C	2.641887	1.850439	0.076613
C	2.627543	3.073269	-0.573968
H	1.368412	4.683580	-1.284452
H	-0.739848	3.553214	-0.610769
C	1.651911	0.070435	1.453320
H	3.593224	1.373198	0.306572
H	3.562550	3.537086	-0.882546
C	-0.454052	-1.159833	1.307244
H	1.215869	0.235935	2.437441
N	-1.065649	1.308337	0.453338
S	-1.193006	-0.224971	0.125979
O	-0.621892	-0.699635	-1.198389
C	-2.965769	-0.405280	-0.052379
C	-3.443332	-1.489886	-0.788393
C	-3.835685	0.452095	0.620289
C	-4.816386	-1.707591	-0.861868
H	-2.743005	-2.139169	-1.310872
C	-5.206560	0.221180	0.539928
H	-3.430613	1.296568	1.173247
C	-5.698680	-0.855541	-0.197873
H	-5.198511	-2.543595	-1.445685
H	-5.894703	0.891911	1.052209
H	-6.771823	-1.029285	-0.257883
C	2.689917	-0.841539	1.399514
C	3.273413	-1.317894	0.192562
H	2.980934	-1.362880	2.308045
O	2.878465	-1.098001	-0.975804
O	4.338649	-2.128356	0.399797
C	4.924481	-2.693175	-0.770685
H	5.301558	-1.909323	-1.435582
H	5.745832	-3.315843	-0.412463
H	4.195632	-3.300458	-1.317695

H	-0.813068	-0.933710	2.311092
H	-0.358411	-2.218795	1.058782
Li	1.209606	-0.436229	-1.378626