IV. Cartesian coordinates of the substrates, products and intermediates by B3LYP/6-31(+)G(d) optimizations

Substrate **2** shown in Figure S1-1
E=-2159.48414630 a.u. and thermal correction=0.515095 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.1219832 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-0.030077	-0.742722	-0.169211
O	0	0.113154	-1.738495	-0.948097
C	0	-0.870560	0.343607	-0.576370
C	0	0.661240	-0.793685	1.133999
C	0	-1.231678	1.523768	0.051364
C	0	0.646862	0.158346	2.145901
C	0	-0.847417	2.019428	1.311942
C	0	-0.008822	1.399311	2.224200
H	0	-1.275625	0.203310	-1.577384
H	0	-1.909275	2.145689	-0.530460
H	0	1.227199	-0.090675	3.024618
H	0	-1.272338	2.976154	1.607250
H	0	0.170098	1.936843	3.151963
C	0	3.717925	0.588903	-0.148630
C	0	2.952819	1.258318	-1.089211
N	0	2.267634	1.900932	-1.810059
C	0	3.775367	1.210608	1.094414
N	0	3.733378	1.807697	2.112203
H	0	4.228390	-0.344964	-0.367977
O	0	1.329693	-1.937435	1.249217
C	0	2.100106	-2.246338	2.425921
H	0	1.437547	-2.290958	3.294799
H	0	2.534106	-3.222760	2.215291
H	0	2.895416	-1.506350	2.556586
H	0	3.045747	3.514507	2.126583
O	0	2.525539	4.290594	1.798533
C	0	2.970036	5.481386	2.453010
H	0	2.803949	5.418085	3.534436
H	0	4.032678	5.666757	2.257722
H	0	2.383823	6.312571	2.052813
H	0	0.901942	3.275207	-2.407481
O	0	0.485409	4.061502	-1.995500
C	0	-0.664576	4.486086	-2.733809
H	0	-0.396876	4.720239	-3.770546
H	0	-1.453727	3.725823	-2.712966
H	0	-1.033683	5.394008	-2.251551
H	0	-1.501565	-2.437628	-1.415822
O	0	-2.476551	-2.568193	-1.459228
C	0	-2.818213	-3.182553	-2.712738
H	0	-2.337505	-2.654780	-3.541673
H	0	-2.515085	-4.235736	-2.716972
H	0	-3.904875	-3.124982	-2.815178
H	0	0.164524	-1.464718	-2.832902
O	0	-0.039263	-1.428150	-3.787845
C	0	1.080585	-0.882435	-4.482104
H	0	1.349908	0.112904	-4.105311
H	0	1.962154	-1.535337	-4.412073
H	0	0.793050	-0.798457	-5.533464
H	0	3.773467	-2.966760	-0.796359
O	0	4.638579	-2.503176	-0.729679
C	0	5.678401	-3.412009	-1.057438
H	0	5.705038	-4.273420	-0.373934
H	0	5.593189	-3.784762	-2.089140
H	0	6.623995	-2.870323	-0.966136
H	0	1.482028	-3.086550	-0.678677
O	0	2.140674	-3.786354	-0.877890
C	0	1.731849	-4.485999	-2.050587
H	0	0.780342	-5.010395	-1.889386
H	0	1.628026	-3.814965	-2.913086
H	0	2.503599	-5.228591	-2.269285
Na	0	1.610277	3.579343	-0.120868

Na	0	-3.423061	-1.291563	0.066632
C	0	-5.308914	0.105503	2.317067
H	0	-6.084825	0.371919	3.020043
C	0	-5.352429	0.415669	0.966072
N	0	-5.235658	0.551179	-0.203398
C	0	-4.221313	-0.698460	2.639053
N	0	-3.265906	-1.388318	2.724229
H	0	-1.574328	-1.784872	3.682820
O	0	-0.781286	-2.013394	4.209581
C	0	-1.190777	-2.841515	5.292238
H	0	-1.891713	-2.323222	5.961197
H	0	-1.657783	-3.772566	4.942488
H	0	-0.292480	-3.095620	5.861976
H	0	-4.277821	1.680986	-1.449739
O	0	-3.639590	2.105173	-2.062565
C	0	-4.199229	2.099156	-3.372076
H	0	-4.430996	1.080495	-3.712614
H	0	-5.111309	2.708612	-3.428534
H	0	-3.451884	2.526455	-4.046418

Transition State, TS(**2** → **3**) shown in Figure S1-2
E=-2159.44929724 a.u. and thermal correction=0.523044 a.u.by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=294.4957i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.081778 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-0.139997	-0.345928	0.731240
O	0	-0.125726	-0.790674	1.929146
C	0	0.959306	0.413915	0.246842
C	0	-1.376490	-0.624229	-0.068941
C	0	1.254714	0.946983	-1.019461
C	0	-1.410156	-0.580427	-1.508223
C	0	0.570153	0.817525	-2.224166
C	0	-0.610375	0.065790	-2.426140
H	0	1.679822	0.655195	1.027528
H	0	2.177213	1.524969	-1.039931
H	0	-2.246353	-1.135655	-1.923023
H	0	1.039559	1.242259	-3.109503
H	0	-0.923924	-0.049346	-3.461544
C	0	-2.654063	0.854946	0.717226
C	0	-1.880060	2.027062	0.948021
N	0	-1.154889	2.940813	1.028633
C	0	-3.600610	1.055244	-0.328571
N	0	-4.232153	1.230469	-1.295768
H	0	-2.983428	0.341749	1.626256
O	0	-2.162293	-1.656112	0.451361
C	0	-1.614887	-2.988026	0.275435
H	0	-0.700410	-3.095878	0.866685
H	0	-2.380833	-3.661730	0.662869
H	0	-1.415115	-3.199226	-0.779648
H	0	-3.215096	2.638578	-2.363822
O	0	-2.556163	3.324986	-2.595885
C	0	-3.208427	4.363774	-3.340488
H	0	-3.619746	3.971384	-4.276711
H	0	-4.007287	4.827407	-2.751374
H	0	-2.451550	5.116985	-3.572135
H	0	0.645233	4.358406	0.482778
O	0	0.855803	4.595728	-0.437369
C	0	2.233170	5.010551	-0.534221
H	0	2.407810	5.897762	0.084152
H	0	2.909812	4.199326	-0.246661
H	0	2.401523	5.274123	-1.580858
H	0	1.346438	-1.836182	2.164799
O	0	2.170614	-2.334753	1.959011
C	0	2.838558	-2.677077	3.183455
H	0	2.964834	-1.790480	3.812067
H	0	2.272713	-3.441903	3.727857
H	0	3.816305	-3.084653	2.914312
H	0	0.826903	0.127119	3.294903
O	0	1.487362	0.432231	3.948096
C	0	0.843734	1.288017	4.888822

H	0	0.494953	2.219372	4.420510
H	0	-0.011020	0.795677	5.370063
H	0	1.585173	1.538326	5.652433
H	0	-4.085553	-1.854176	0.625891
O	0	-4.996743	-2.091470	0.877049
C	0	-5.785281	-2.239232	-0.299631
H	0	-5.841433	-1.306315	-0.876936
H	0	-5.407759	-3.040252	-0.951853
H	0	-6.792680	-2.508015	0.027892
H	0	-1.707018	-0.849502	3.006514
O	0	-2.444214	-0.496338	3.544612
C	0	-3.232975	-1.572052	4.050944
H	0	-3.715437	-2.140820	3.246314
H	0	-2.635873	-2.252859	4.673814
H	0	-4.011656	-1.126464	4.674956
Na	0	-0.625571	3.226625	-1.413003
Na	0	2.779151	-1.772342	-0.095967
C	0	4.741998	-1.867719	-2.701248
H	0	5.491148	-2.066784	-3.453885
C	0	4.926937	-0.981764	-1.648734
N	0	4.926156	-0.302409	-0.681309
C	0	3.540431	-2.559488	-2.611605
N	0	2.499703	-3.061835	-2.365482
H	0	0.607379	-3.470393	-2.721785
O	0	-0.329767	-3.717856	-2.860593
C	0	-0.365268	-4.947812	-3.573941
H	0	0.096844	-4.859449	-4.567328
H	0	0.134789	-5.757476	-3.023710
H	0	-1.417605	-5.214949	-3.704947
H	0	4.464652	1.431785	0.045713
O	0	4.062794	2.240014	0.430244
C	0	4.454378	2.332595	1.798989
H	0	4.052971	1.504390	2.398106
H	0	5.546956	2.361342	1.906520
H	0	4.043567	3.268038	2.189897

A Meisenheimer intermediate **3** shown in Figure S1-3
E=-2159.50092014 a.u. and thermal correction=0.531178 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.1249315 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-2.180415	-2.193674	-0.430404
O	0	-3.250528	-1.961531	0.258438
C	0	-1.985452	-3.401644	-1.087214
C	0	-1.208896	-0.995068	-0.435449
C	0	-0.932576	-3.890887	-1.900111
C	0	0.125354	-1.069239	-1.090373
C	0	0.250207	-3.306780	-2.278267
C	0	0.701644	-2.012922	-1.893414
H	0	-2.821006	-4.084629	-0.948976
H	0	-1.107439	-4.895389	-2.283408
H	0	0.683755	-0.137061	-0.985795
H	0	0.911399	-3.875659	-2.926059
H	0	1.670089	-1.713693	-2.295247
C	0	-1.091051	-0.584063	1.126380
C	0	-0.867026	0.840034	1.360195
N	0	-0.752199	1.985670	1.515347
C	0	-0.052961	-1.385741	1.774613
N	0	0.794028	-2.034394	2.231533
H	0	-2.081385	-0.846946	1.533542
O	0	-1.933328	0.174202	-0.980717
C	0	-2.392261	-0.019713	-2.330034
H	0	-3.081379	-0.867019	-2.390117
H	0	-2.929602	0.891698	-2.605309
H	0	-1.546840	-0.181551	-3.007356
H	0	0.362860	3.773518	1.607800
O	0	0.897570	4.586810	1.616766
C	0	0.627722	5.298317	2.821945
H	0	-0.431513	5.578586	2.905214
H	0	0.913268	4.721598	3.712515

H	0	1.227812	6.210923	2.792081
H	0	2.406516	1.512727	0.856581
O	0	2.393318	0.761295	1.492959
C	0	2.706892	1.221114	2.809522
H	0	3.724717	1.627833	2.858003
H	0	1.995006	1.987213	3.139035
H	0	2.637565	0.358961	3.477004
H	0	-4.267371	-0.525799	0.177019
O	0	-4.934070	0.207470	0.202641
C	0	-6.229661	-0.329487	-0.094560
H	0	-6.357150	-0.484690	-1.174146
H	0	-6.380344	-1.281814	0.422578
H	0	-6.972101	0.395390	0.250995
H	0	-4.588155	-3.134614	0.578183
O	0	-5.388968	-3.672027	0.775102
C	0	-5.153438	-4.427529	1.952320
H	0	-4.304592	-5.118787	1.840251
H	0	-4.966457	-3.787261	2.827795
H	0	-6.053114	-5.018930	2.145890
H	0	0.924353	3.089561	-1.276662
O	0	0.055745	3.462017	-1.568096
C	0	0.248540	4.837282	-1.921023
H	0	0.570078	5.421046	-1.051467
H	0	0.982329	4.933392	-2.730008
H	0	-0.711313	5.220643	-2.279506
H	0	-4.380853	1.717790	-0.337507
O	0	-4.015001	2.607777	-0.607454
C	0	-5.001684	3.609487	-0.363704
H	0	-5.286118	3.638954	0.695441
H	0	-4.571164	4.576225	-0.640594
H	0	-5.897495	3.438798	-0.973331
Na	0	-1.787789	2.495047	-0.733194
Na	0	2.771375	-1.258078	0.488281
C	0	5.725068	-1.057891	-2.105441
H	0	6.063932	-1.224806	-3.120048
C	0	6.403274	-1.605440	-1.012615
N	0	6.893497	-2.061119	-0.044772
C	0	4.529373	-0.431912	-1.848985
N	0	3.487173	0.062893	-1.565161
H	0	2.892573	1.680904	-1.163384
O	0	2.512642	2.477913	-0.694539
C	0	3.527156	3.490411	-0.576828
H	0	4.438515	3.071799	-0.134630
H	0	3.768538	3.914932	-1.558158
H	0	3.125045	4.266573	0.076936
H	0	5.268551	-2.600405	0.890907
O	0	4.350250	-2.676365	1.236361
C	0	4.277085	-3.771290	2.155551
H	0	4.511078	-4.719046	1.656247
H	0	4.965420	-3.622881	2.995780
H	0	3.252652	-3.806792	2.533005

Transition State, TS(**3** → **4**) shown in Figure S1-4
E=-2159.481514 a.u. and thermal correction=0.525508 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=238.2813i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.108945 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	2.031908	-2.024974	0.787010
O	0	2.688907	-2.275235	-0.289965
C	0	2.124138	-2.908734	1.885799
C	0	1.230978	-0.769375	0.799273
C	0	1.507152	-2.910017	3.137755
C	0	0.220994	-0.443983	1.745468
C	0	0.557108	-2.044629	3.669050
C	0	-0.026023	-0.955179	3.011519
H	0	2.808285	-3.732236	1.693345
H	0	1.810582	-3.731108	3.785249
H	0	-0.434616	0.376156	1.453789
H	0	0.197926	-2.260911	4.671534
H	0	-0.826349	-0.450310	3.549710

C	0	0.907112	-0.349303	-0.666701
C	0	0.871024	1.093976	-0.914925
N	0	0.893588	2.229485	-1.155197
C	0	-0.359736	-0.956710	-1.105854
N	0	-1.359396	-1.440528	-1.436856
H	0	1.718451	-0.784771	-1.271185
O	0	2.598409	0.558729	0.996020
C	0	3.544087	0.148610	1.965023
H	0	4.175116	-0.679145	1.612059
H	0	4.208175	0.993738	2.202813
H	0	3.056291	-0.160450	2.901323
H	0	-0.381057	3.853904	-0.809461
O	0	-0.934279	4.623919	-0.589588
C	0	-0.499811	5.733434	-1.368716
H	0	0.542053	6.008986	-1.149051
H	0	-0.596458	5.543277	-2.446655
H	0	-1.142829	6.576721	-1.105307
H	0	-2.832284	1.765995	-0.454607
O	0	-3.089428	1.428974	-1.348834
C	0	-3.622964	2.495466	-2.135747
H	0	-4.593362	2.833519	-1.748444
H	0	-2.930782	3.344462	-2.162503
H	0	-3.764054	2.112255	-3.149877
H	0	4.078953	-1.398580	-1.002653
O	0	4.852756	-1.001440	-1.468711
C	0	6.011154	-1.812487	-1.225338
H	0	6.403769	-1.648553	-0.213271
H	0	5.771424	-2.872307	-1.353044
H	0	6.770895	-1.518428	-1.954263
H	0	3.497448	-3.888260	-0.577689
O	0	4.030552	-4.702483	-0.712588
C	0	3.294179	-5.607857	-1.522406
H	0	2.342083	-5.900769	-1.055985
H	0	3.082020	-5.194014	-2.519228
H	0	3.907105	-6.505174	-1.645086
H	0	2.078285	2.271940	1.823512
O	0	2.398555	3.199544	1.763285
C	0	1.468801	4.107685	2.364229
H	0	0.513444	4.117688	1.827294
H	0	1.301955	3.855343	3.417886
H	0	1.919048	5.101493	2.309342
H	0	4.920068	0.693713	-1.495507
O	0	4.890737	1.689915	-1.538250
C	0	5.670211	2.133138	-2.649304
H	0	5.301031	1.704840	-3.589008
H	0	5.587764	3.222427	-2.700680
H	0	6.726730	1.867704	-2.521511
Na	0	3.300868	2.415669	-0.172545
Na	0	-3.685024	-0.749455	-1.003226
C	0	-6.210680	-1.723484	1.729117
H	0	-6.419759	-2.367109	2.573908
C	0	-7.057567	-1.678248	0.620969
N	0	-7.693206	-1.611952	-0.368820
C	0	-5.010482	-1.056529	1.618124
N	0	-3.984531	-0.490555	1.435846
H	0	-3.025186	1.064351	1.527505
O	0	-2.465579	1.843567	1.281719
C	0	-2.937574	3.014589	1.954355
H	0	-4.011952	3.166074	1.787703
H	0	-2.752192	2.948647	3.034070
H	0	-2.388339	3.863014	1.540533
H	0	-6.271750	-1.703494	-1.662038
O	0	-5.413112	-1.666528	-2.146385
C	0	-5.534969	-2.396580	-3.368462
H	0	-5.784618	-3.447372	-3.178586
H	0	-6.299728	-1.953016	-4.016965
H	0	-4.567435	-2.348294	-3.875366

A neutral intermediate **4** shown in Figure S1-5
E=-2159.52341154 a.u. and thermal correction=0.525992 a.u. by B3LYP/6-31(+)G(d)

SCRF=(PCM, solvent=methanol)=-2160.145152 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	1.488528	2.602008	0.306173
O	0	0.321638	2.280035	0.670758
C	0	2.022953	3.857437	0.795074
C	0	2.207896	1.723051	-0.613288
C	0	3.270282	4.408044	0.687948
C	0	3.528397	1.789217	-0.978845
C	0	4.435317	3.895549	0.055593
C	0	4.545224	2.732097	-0.656846
H	0	1.286579	4.418484	1.366303
H	0	3.395784	5.369110	1.182664
H	0	3.893017	0.980273	-1.604200
H	0	5.335112	4.496979	0.158446
H	0	5.523764	2.470224	-1.045615
C	0	1.380717	0.506975	-1.083536
C	0	2.006771	-0.252531	-2.177708
N	0	2.482153	-0.818923	-3.071051
C	0	0.010533	0.838424	-1.522435
N	0	-1.077460	1.013281	-1.883931
H	0	1.259778	-0.166866	-0.202623
O	0	0.995817	-1.183614	1.532440
C	0	1.612930	-0.707351	2.721314
H	0	1.137381	0.236400	3.010773
H	0	1.498166	-1.422568	3.548598
H	0	2.685053	-0.523895	2.568514
O	0	2.142157	-3.064680	0.342453
C	0	2.143585	-4.306978	1.009209
H	0	1.160946	-4.526249	1.466512
H	0	2.370807	-5.133642	0.317358
H	0	2.894579	-4.335902	1.815282
H	0	3.639786	-2.682108	-0.170264
O	0	4.576996	-2.476383	-0.489620
C	0	4.836084	-3.210497	-1.680391
H	0	4.747695	-4.291940	-1.507315
H	0	4.156230	-2.920380	-2.491726
H	0	5.863323	-2.994243	-1.990374
H	0	0.859167	-2.840928	-0.578806
O	0	-0.036302	-2.524488	-0.951102
C	0	-0.353819	-3.220570	-2.150734
H	0	0.381084	-3.009286	-2.938132
H	0	-0.396278	-4.306502	-1.986501
H	0	-1.338654	-2.881710	-2.486405
H	0	-1.014893	1.100321	1.089581
O	0	-1.838519	0.583007	1.215303
C	0	-2.331082	0.807413	2.552843
H	0	-1.639056	0.388748	3.291855
H	0	-2.466977	1.877367	2.739719
H	0	-3.287698	0.287674	2.630788
H	0	-0.783344	3.572611	1.483398
O	0	-1.284369	4.268264	1.954597
C	0	-2.304397	4.772116	1.100943
H	0	-1.896017	5.194783	0.171343
H	0	-3.045451	4.000614	0.843018
H	0	-2.814756	5.569268	1.647121
H	0	5.339329	-0.927720	-0.319302
O	0	5.819986	-0.065823	-0.221041
C	0	7.011179	-0.306012	0.513674
H	0	6.803173	-0.730068	1.506040
H	0	7.693176	-0.984332	-0.018861
H	0	7.518789	0.654892	0.647702
H	0	1.551708	-1.989688	1.133077
Na	0	-1.161123	-1.771542	0.881320
Na	0	-3.149508	0.558734	-0.718645
C	0	-5.784404	-1.933899	-1.344066
H	0	-6.022984	-2.710697	-2.059568
C	0	-4.583210	-1.926998	-0.676388
N	0	-3.549064	-1.839503	-0.097636
C	0	-6.618813	-0.826426	-1.168171
N	0	-7.240924	0.157844	-0.997782

H	0	-5.804303	1.438465	-1.146142
O	0	-4.921566	1.874887	-1.193611
C	0	-5.046075	3.099742	-1.922692
H	0	-5.423607	2.919285	-2.936072
H	0	-5.713372	3.797278	-1.403599
H	0	-4.048676	3.541992	-1.988835
H	0	-3.269126	-2.732004	1.679689
O	0	-2.573694	-2.851503	2.360804
C	0	-2.807697	-4.033421	3.125842
H	0	-3.750588	-3.965985	3.682298
H	0	-2.823467	-4.928483	2.490930
H	0	-1.983712	-4.119535	3.837781

Transition State, TS(**4** → **5**) shown in Figure S1-6
E=-2159.52272586 a.u. and thermal correction=0.525854 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=421.8106i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.143576 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	1.426674	2.668321	0.263520
O	0	0.254786	2.356977	0.622252
C	0	1.952111	3.940690	0.715613
C	0	2.162201	1.756577	-0.611320
C	0	3.200726	4.489823	0.610129
C	0	3.489142	1.814430	-0.957788
C	0	4.376209	3.958556	0.015105
C	0	4.498348	2.770314	-0.654278
H	0	1.206932	4.519377	1.257058
H	0	3.316541	5.467386	1.073979
H	0	3.868188	0.984462	-1.546259
H	0	5.273349	4.565194	0.110483
H	0	5.482390	2.496224	-1.020576
C	0	1.349628	0.522126	-1.043347
C	0	1.993223	-0.285862	-2.088593
N	0	2.480507	-0.912941	-2.934358
C	0	-0.016347	0.817590	-1.508380
N	0	-1.107816	0.948706	-1.879887
H	0	1.225639	-0.125596	-0.116604
O	0	1.021801	-1.106957	1.399972
C	0	1.580449	-0.514073	2.557855
H	0	1.090764	0.448244	2.762069
H	0	1.447972	-1.154080	3.444592
H	0	2.658583	-0.326228	2.438200
O	0	2.222969	-3.007896	0.509430
C	0	2.245235	-4.125187	1.379537
H	0	1.239600	-4.348307	1.774128
H	0	2.598565	-5.016249	0.843627
H	0	2.915908	-3.958297	2.235899
H	0	3.774495	-2.671819	-0.063498
O	0	4.701475	-2.522035	-0.410189
C	0	4.878281	-3.283857	-1.601332
H	0	4.740676	-4.356619	-1.409246
H	0	4.186116	-2.965886	-2.390725
H	0	5.904038	-3.124103	-1.946677
H	0	0.870700	-2.987802	-0.510520
O	0	-0.040474	-2.766116	-0.862606
C	0	-0.302807	-3.478099	-2.067624
H	0	0.411451	-3.203432	-2.854016
H	0	-0.261894	-4.564548	-1.909386
H	0	-1.311388	-3.210594	-2.394698
H	0	-1.057672	1.146087	1.057710
O	0	-1.869377	0.614393	1.201088
C	0	-2.336115	0.833412	2.548408
H	0	-1.621081	0.427639	3.272382
H	0	-2.485541	1.901482	2.736395
H	0	-3.282204	0.298511	2.648401
H	0	-0.843872	3.643768	1.442380
O	0	-1.345882	4.337218	1.916378
C	0	-2.381790	4.825250	1.073642
H	0	-1.990647	5.243923	0.134757
H	0	-3.119849	4.045399	0.832310

H	0	-2.891695	5.622391	1.620390
H	0	5.422922	-0.920960	-0.389109
O	0	5.886774	-0.046587	-0.372718
C	0	7.150374	-0.231130	0.249436
H	0	7.051069	-0.615530	1.274147
H	0	7.793078	-0.917490	-0.320318
H	0	7.644837	0.744757	0.292341
H	0	1.670935	-2.036582	1.040324
Na	0	-1.124954	-1.748023	0.870700
Na	0	-3.188046	0.535415	-0.722302
C	0	-5.721583	-2.052957	-1.394499
H	0	-5.925750	-2.842229	-2.106964
C	0	-4.530308	-2.002477	-0.711001
N	0	-3.507577	-1.877709	-0.119070
C	0	-6.594748	-0.973137	-1.235740
N	0	-7.252086	-0.009968	-1.077542
H	0	-5.864721	1.323938	-1.182628
O	0	-4.999757	1.796803	-1.198205
C	0	-5.169462	3.057270	-1.853217
H	0	-5.520606	2.922882	-2.883140
H	0	-5.877563	3.689995	-1.305880
H	0	-4.193284	3.548721	-1.872054
H	0	-3.224810	-2.704549	1.683007
O	0	-2.541217	-2.794167	2.380768
C	0	-2.763203	-3.968739	3.159853
H	0	-3.721395	-3.917922	3.691539
H	0	-2.739308	-4.874736	2.540589
H	0	-1.955879	-4.020861	3.893968

The monoanion **5** shown in Figure S1-7
E=-2159.54719598 a.u. and thermal correction=0.521905 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.174848 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-1.854190	2.539125	-0.179289
O	0	-2.551293	1.464505	-0.053620
C	0	-2.526095	3.788719	-0.159205
C	0	-0.405257	2.367093	-0.350642
C	0	-2.070210	5.099403	-0.246807
C	0	0.535214	3.413856	-0.435905
C	0	-0.766256	5.575784	-0.371643
C	0	0.389277	4.799161	-0.444247
H	0	-3.602947	3.666120	-0.062251
H	0	-2.850824	5.857353	-0.206195
H	0	1.577190	3.106875	-0.481485
H	0	-0.637760	6.654499	-0.409107
H	0	1.334046	5.333543	-0.514284
C	0	0.075495	1.018673	-0.417947
C	0	-0.650327	-0.164928	-0.163345
N	0	-1.030272	-1.260463	0.025734
C	0	1.429829	0.744368	-0.709349
N	0	2.540402	0.478670	-0.956871
H	0	-2.422985	-2.193751	0.741864
O	0	-3.228552	-2.547843	1.191564
C	0	-2.987334	-2.546784	2.605670
H	0	-2.819438	-1.527392	2.968600
H	0	-2.127599	-3.178424	2.855960
H	0	-3.881015	-2.954950	3.085711
H	0	2.918767	-1.976053	1.280906
O	0	3.747771	-1.518592	1.560557
C	0	4.482635	-2.393086	2.427020
H	0	3.887650	-2.650854	3.311720
H	0	4.787262	-3.303149	1.899023
H	0	5.374999	-1.850553	2.751701
H	0	0.668351	-2.432705	0.557595
O	0	1.514454	-2.902101	0.682941
C	0	1.813085	-3.653017	-0.506250
H	0	1.120901	-4.497380	-0.612534
H	0	1.754123	-3.018086	-1.398657
H	0	2.834767	-4.025087	-0.404435

H	0	-3.733999	0.984371	1.171703
O	0	-4.458760	0.542216	1.677952
C	0	-5.189815	1.521806	2.410988
H	0	-4.552128	2.023433	3.149638
H	0	-5.636105	2.275203	1.748098
H	0	-5.993732	1.002669	2.939813
H	0	-3.495608	0.538894	-1.180262
O	0	-4.117445	-0.096181	-1.617215
C	0	-3.455146	-0.740654	-2.713699
H	0	-3.180142	-0.014843	-3.487948
H	0	-2.559356	-1.268356	-2.370040
H	0	-4.160648	-1.460792	-3.136532
H	0	-4.586746	-3.633331	0.440783
O	0	-5.493580	-3.468460	0.110563
C	0	-6.080218	-4.649150	-0.432775
H	0	-5.488850	-5.043776	-1.268548
H	0	-6.192279	-5.427989	0.331540
H	0	-7.070336	-4.371485	-0.800879
H	0	-6.005169	0.199571	-1.512692
O	0	-6.746572	-0.098659	-0.947026
C	0	-8.002664	0.321432	-1.472269
H	0	-8.773191	-0.054536	-0.795394
H	0	-8.074930	1.415648	-1.515600
H	0	-8.180483	-0.092458	-2.473043
Na	0	-5.106770	-1.201426	0.303524
Na	0	4.575150	-0.145521	-0.011031
C	0	7.625342	0.675458	-0.900261
H	0	8.631901	0.940497	-1.191249
C	0	6.735795	1.584644	-0.342717
N	0	5.880470	2.236495	0.146162
C	0	7.106759	-0.604214	-1.052827
N	0	6.531481	-1.633221	-1.120525
H	0	5.736641	-3.357942	-0.710364
O	0	5.319322	-4.215311	-0.481505
C	0	6.149226	-5.258833	-0.971687
H	0	6.255268	-5.221193	-2.065375
H	0	7.151777	-5.233445	-0.521012
H	0	5.673425	-6.206292	-0.701907
H	0	4.413547	3.525547	0.133717
O	0	3.673236	4.143564	0.313907
C	0	3.866028	4.669466	1.619979
H	0	3.924846	3.875515	2.377908
H	0	4.775439	5.283285	1.684998
H	0	3.002936	5.302817	1.847881

Transition State, TS(**5** → **6**) shown in Figure S1-8
E=-2159.50932362 a.u. and thermal correction=0.520781 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=689.8939i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.140924 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-2.080534	2.149621	-0.263922
O	0	-2.334053	0.826438	-0.059999
C	0	-3.127114	3.034342	-0.353090
C	0	-0.653529	2.363982	-0.376605
C	0	-3.051169	4.434697	-0.564908
C	0	0.001257	3.620122	-0.525692
C	0	-1.942211	5.238653	-0.699934
C	0	-0.572106	4.861608	-0.664387
H	0	-4.129306	2.614807	-0.282179
H	0	-4.017253	4.930388	-0.624710
H	0	1.090504	3.599733	-0.500964
H	0	-2.131803	6.299060	-0.847404
H	0	0.137767	5.679603	-0.765351
C	0	-0.033137	1.120726	-0.286118
C	0	-0.968490	0.031828	-0.064181
N	0	-0.912903	-1.185544	0.101102
C	0	1.346383	0.877988	-0.399018
N	0	2.485109	0.656491	-0.504111
H	0	-1.801934	-1.946548	0.367386
O	0	-2.689259	-2.833175	0.760186

C	0	-2.128816	-3.533387	1.854036
H	0	-1.839430	-2.850679	2.670539
H	0	-1.229261	-4.095921	1.562043
H	0	-2.854143	-4.252080	2.268484
H	0	2.909051	-1.983909	1.219512
O	0	3.733101	-1.610378	1.625914
C	0	4.427548	-2.664263	2.303418
H	0	3.791982	-3.111080	3.077794
H	0	4.758290	-3.434985	1.598463
H	0	5.303937	-2.219611	2.783859
H	0	0.723308	-2.176770	0.312958
O	0	1.554883	-2.703457	0.386284
C	0	1.894817	-3.215015	-0.907948
H	0	1.194441	-4.004626	-1.209604
H	0	1.886889	-2.419331	-1.664079
H	0	2.904539	-3.627727	-0.845824
H	0	-3.602577	0.388689	1.417675
O	0	-4.362763	0.005220	1.896892
C	0	-4.095802	0.042994	3.305549
H	0	-3.212618	-0.554601	3.559606
H	0	-3.955956	1.073659	3.650574
H	0	-4.970867	-0.378480	3.805599
H	0	-5.714112	0.954419	-1.197320
O	0	-6.169554	1.802250	-1.024054
C	0	-7.338711	1.551546	-0.251442
H	0	-8.045267	0.894646	-0.778464
H	0	-7.095296	1.110669	0.726257
H	0	-7.825943	2.515463	-0.085224
H	0	-3.808254	-3.803675	-0.090093
O	0	-4.758329	-3.928078	-0.386487
C	0	-4.987970	-5.231672	-0.906024
H	0	-4.353349	-5.433290	-1.778824
H	0	-4.807657	-6.005627	-0.148502
H	0	-6.035143	-5.284305	-1.215977
H	0	-3.668199	-0.022245	-1.071340
O	0	-4.486563	-0.499405	-1.326049
C	0	-4.299289	-1.111189	-2.618018
H	0	-4.156567	-0.346266	-3.388793
H	0	-3.444139	-1.793832	-2.600743
H	0	-5.206137	-1.678584	-2.831462
Na	0	-4.703359	-1.864104	0.573513
Na	0	4.566936	0.009614	0.333627
C	0	7.434565	1.363131	-0.531613
H	0	8.422724	1.759473	-0.717767
C	0	6.406208	2.123384	0.009488
N	0	5.453762	2.640301	0.480117
C	0	7.096524	0.036818	-0.768943
N	0	6.666888	-1.054553	-0.904921
H	0	5.920051	-2.861994	-0.925445
O	0	5.503621	-3.748481	-0.912729
C	0	6.342366	-4.645713	-1.625875
H	0	6.475546	-4.340914	-2.673934
H	0	7.333752	-4.741930	-1.159862
H	0	5.856764	-5.625830	-1.609433
H	0	3.852561	3.708590	0.240019
O	0	3.080778	4.316477	0.262188
C	0	3.358111	5.323549	1.226097
H	0	3.551413	4.896841	2.219939
H	0	4.218819	5.941905	0.935601
H	0	2.475247	5.967638	1.290741

The key intermediate **6** shown in Figure S1-9
E=-2159.53206517 a.u. and thermal correction=0.526104 a.u. by B3LYP/6-31G(d)
SCRF=(PCM, solvent=methanol)=-2160.164973 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	0.415240	2.599376	-1.017155
O	0	0.629070	1.298514	-0.678501
C	0	1.494672	3.438500	-1.125428
C	0	-0.997029	2.804220	-1.226256

C	0	1.447201	4.811531	-1.458248
C	0	-1.615438	4.024982	-1.600266
C	0	0.358057	5.603331	-1.761325
C	0	-1.012540	5.240768	-1.826598
H	0	2.470416	3.010442	-0.904626
H	0	2.415664	5.305586	-1.467825
H	0	-2.696472	3.984295	-1.711291
H	0	0.572373	6.645835	-1.982840
H	0	-1.688702	6.049056	-2.096940
C	0	-1.607103	1.565704	-1.002522
C	0	-0.588192	0.610201	-0.633731
N	0	-0.657089	-0.627518	-0.319295
C	0	-2.977799	1.268035	-1.102043
N	0	-4.114869	1.026167	-1.202679
H	0	0.267906	-1.002841	-0.062660
O	0	1.786025	-1.744974	1.090379
C	0	2.546443	-0.682713	1.680358
H	0	3.083558	-0.107721	0.917954
H	0	1.852835	-0.008584	2.187670
H	0	3.265480	-1.071420	2.413146
H	0	-5.535759	-0.244020	-1.818786
O	0	-6.111357	-0.972518	-2.119199
C	0	-7.451668	-0.503193	-2.178352
H	0	-7.818318	-0.175187	-1.195043
H	0	-7.567767	0.324467	-2.892747
H	0	-8.068978	-1.339955	-2.516020
H	0	-2.034285	-2.084906	-0.943503
O	0	-2.527081	-2.812837	-0.513584
C	0	-3.563811	-3.317203	-1.366412
H	0	-4.304700	-2.549013	-1.610628
H	0	-3.141471	-3.733893	-2.289533
H	0	-4.055162	-4.121514	-0.813764
H	0	2.021529	-4.219285	-0.916359
O	0	1.546432	-4.517783	-1.746291
C	0	0.299799	-5.151096	-1.457557
H	0	0.450726	-6.061457	-0.864277
H	0	-0.379515	-4.475751	-0.924462
H	0	-0.152377	-5.428418	-2.413481
H	0	4.263071	-2.014764	-1.037941
O	0	4.501136	-1.599354	-1.913972
C	0	5.246102	-0.388309	-1.757269
H	0	4.714708	0.335420	-1.129389
H	0	6.233639	-0.592361	-1.324755
H	0	5.382632	0.036449	-2.755233
H	0	2.412678	-2.372370	0.586550
O	0	3.355455	-3.320826	-0.256325
C	0	4.162557	-4.131240	0.571958
H	0	3.954644	-3.958375	1.640906
H	0	3.997226	-5.205636	0.380392
H	0	5.237117	-3.935585	0.414570
H	0	0.546465	-2.415054	2.088982
O	0	-0.288866	-2.676849	2.557142
C	0	-0.032851	-2.831643	3.952280
H	0	0.693843	-3.633757	4.134499
H	0	0.335422	-1.899760	4.399953
H	0	-0.977985	-3.099513	4.431866
H	0	-0.547531	4.430526	2.476157
C	0	-0.169087	3.414263	2.480610
C	0	1.199385	3.205565	2.367613
N	0	2.361744	3.052710	2.246115
C	0	-1.054070	2.373356	2.729775
N	0	-1.827677	1.507261	2.924010
H	0	-3.023936	0.182216	2.904092
O	0	-3.544829	-0.642764	2.723282
C	0	-4.919439	-0.307251	2.546400
H	0	-5.342474	0.115666	3.466317
H	0	-5.055684	0.404884	1.722602
H	0	-5.454727	-1.229981	2.305520
H	0	3.672271	2.650653	1.019760
O	0	4.310328	2.486932	0.281654
C	0	5.569230	3.031045	0.653689

H	0	5.512165	4.113828	0.835043
H	0	5.973191	2.548257	1.554431
H	0	6.262178	2.854908	-0.175080
Na	0	-2.045829	-1.754816	1.472445
Na	0	3.152273	-3.224405	-2.543724

Transition State, TS(**6** → **16**) shown in Figure S2-1
E=-2159.54207859 a.u. and thermal correction=0.534361 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=289.9836i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.153765 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	2.241656	-2.278411	0.329728
O	0	0.862671	-2.133883	0.388436
C	0	2.798907	-3.477086	0.782538
C	0	2.808526	-1.116725	-0.207445
C	0	4.117183	-3.867684	0.625801
C	0	4.218550	-0.818941	-0.298490
C	0	5.154045	-3.163812	-0.038875
C	0	5.192095	-1.864084	-0.496141
H	0	2.103671	-4.175405	1.241596
H	0	4.369114	-4.860098	0.989984
H	0	4.436463	0.091211	-0.851707
H	0	6.058936	-3.742369	-0.216364
H	0	6.106350	-1.546009	-0.993078
C	0	1.724348	-0.250324	-0.522801
C	0	0.516598	-0.895932	-0.115484
N	0	-0.713308	-0.469732	-0.136786
C	0	1.745348	1.049894	-1.040149
N	0	1.680197	2.139103	-1.465882
H	0	-1.359630	-1.129613	0.304270
O	0	-3.339402	-1.218965	1.653420
C	0	-3.136912	-1.636451	2.999625
H	0	-3.010965	-2.725252	3.057553
H	0	-2.223868	-1.161077	3.372069
H	0	-3.975728	-1.343507	3.646190
H	0	0.357808	3.517435	-1.000168
O	0	-0.518606	3.811728	-0.673454
C	0	-1.101704	4.701141	-1.625295
H	0	-0.502108	5.613144	-1.733467
H	0	-1.216408	4.223863	-2.606782
H	0	-2.090149	4.973957	-1.246656
H	0	-1.492010	0.300848	-1.561767
O	0	-2.089422	0.852955	-2.140916
C	0	-1.533127	0.952427	-3.453417
H	0	-0.520044	1.370370	-3.420585
H	0	-1.506104	-0.025671	-3.951068
H	0	-2.174057	1.623710	-4.031524
H	0	-6.142107	-0.648092	-0.045687
O	0	-6.313176	0.236236	-0.525305
C	0	-7.533970	0.151379	-1.250189
H	0	-7.510068	-0.660379	-1.991200
H	0	-8.387864	-0.008760	-0.578428
H	0	-7.683825	1.101008	-1.774249
H	0	-4.764575	-2.175261	-0.921699
O	0	-4.256610	-1.945563	-1.770777
C	0	-3.339937	-2.980849	-2.092402
H	0	-2.667364	-3.204816	-1.252329
H	0	-3.862442	-3.903196	-2.381670
H	0	-2.735210	-2.647068	-2.941455
H	0	-4.226979	-1.614187	1.274728
O	0	-5.473235	-1.995315	0.509970
C	0	-6.305752	-2.998991	1.040107
H	0	-6.807952	-2.667580	1.964626
H	0	-7.093977	-3.288410	0.325436
H	0	-5.738780	-3.913205	1.284020
H	0	-3.391468	0.378721	1.270111
O	0	-3.415871	1.281623	0.824780
C	0	-4.380658	2.107813	1.495737

H	0	-5.386300	1.688100	1.391798
H	0	-4.126491	2.221188	2.556881
H	0	-4.356932	3.092529	1.019740
C	0	4.732865	0.041324	1.568428
H	0	4.872634	-0.899668	2.098607
C	0	5.950283	0.728544	1.292553
N	0	6.955882	1.219998	0.960206
C	0	3.651617	0.811227	2.083519
N	0	2.706155	1.375491	2.469657
H	0	7.755243	0.476880	-0.773291
O	0	7.857287	-0.075598	-1.571352
C	0	8.816806	0.523758	-2.434811
H	0	8.506207	1.526249	-2.760179
H	0	9.806139	0.593263	-1.961948
H	0	8.896801	-0.118526	-3.315636
H	0	0.907011	1.988585	2.411014
O	0	0.011478	2.382847	2.322503
C	0	0.052124	3.690680	2.898545
H	0	0.303409	3.642091	3.964902
H	0	0.774647	4.332640	2.380604
H	0	-0.944908	4.126667	2.790555
Na	0	-1.199766	1.878759	0.438264
Na	0	-4.135949	0.275765	-1.275451

The anion adduct **16** shown in Figure S2-2
E=-2159.55607492 a.u. and thermal correction=0.534976 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.166146 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	2.375107	-2.164316	0.126701
O	0	0.981282	-2.124287	0.025516
C	0	2.995195	-3.355454	0.571544
C	0	2.897545	-0.951335	-0.266034
C	0	4.320762	-3.667257	0.391124
C	0	4.330176	-0.564529	-0.095039
C	0	5.281618	-2.907190	-0.368869
C	0	5.266377	-1.587905	-0.691547
H	0	2.341087	-4.093226	1.030495
H	0	4.646454	-4.644128	0.739501
H	0	4.507352	0.409299	-0.560220
H	0	6.114906	-3.486791	-0.765079
H	0	6.031151	-1.201082	-1.359635
C	0	1.796038	-0.132189	-0.670513
C	0	0.605724	-0.885969	-0.440279
N	0	-0.652636	-0.540385	-0.561701
C	0	1.787496	1.195850	-1.102625
N	0	1.712142	2.309215	-1.464727
H	0	-1.280411	-1.298587	-0.277812
O	0	-4.339891	-0.169297	2.406647
C	0	-5.112011	0.263464	3.517829
H	0	-5.279231	-0.560658	4.223320
H	0	-4.554424	1.050490	4.035694
H	0	-6.088149	0.665899	3.209955
H	0	0.217595	3.426967	-1.017143
O	0	-0.703907	3.638099	-0.749592
C	0	-1.338893	4.343516	-1.816374
H	0	-0.798375	5.267126	-2.056335
H	0	-1.418000	3.722386	-2.717362
H	0	-2.344075	4.606209	-1.476437
H	0	-1.423041	0.128606	-2.009394
O	0	-2.127641	0.485839	-2.626794
C	0	-1.626128	0.555855	-3.958881
H	0	-0.739370	1.199811	-4.015436
H	0	-1.369341	-0.439393	-4.345279
H	0	-2.412382	0.984701	-4.586536
H	0	-6.049311	-0.985545	-0.298287
O	0	-6.120709	-0.340527	-1.091204
C	0	-7.397488	-0.434683	-1.701868
H	0	-7.588847	-1.444065	-2.093663

H	0	-8.200119	-0.173955	-0.998317
H	0	-7.429625	0.272175	-2.537367
H	0	-4.143891	-2.246070	0.113184
O	0	-3.320681	-2.218796	-0.493029
C	0	-3.119286	-3.490681	-1.096443
H	0	-2.905811	-4.260650	-0.343427
H	0	-3.993965	-3.804635	-1.684513
H	0	-2.257260	-3.415228	-1.766861
H	0	-4.843738	-0.900261	1.880771
O	0	-5.486629	-1.878481	0.879934
C	0	-6.236692	-2.939009	1.422299
H	0	-7.148182	-2.577890	1.927763
H	0	-6.557291	-3.651496	0.643329
H	0	-5.654472	-3.508977	2.165592
H	0	-3.820352	0.844391	1.263955
O	0	-3.522989	1.405522	0.474882
C	0	-4.431509	2.509137	0.357844
H	0	-5.455319	2.151114	0.198336
H	0	-4.400264	3.142323	1.253584
H	0	-4.122624	3.105542	-0.505288
C	0	4.652356	-0.386436	1.468477
H	0	4.580666	-1.387107	1.915884
C	0	6.019396	0.113764	1.656919
N	0	7.112384	0.498079	1.725405
C	0	3.669560	0.479759	2.133373
N	0	2.844708	1.137732	2.614817
H	0	8.067983	0.415010	-0.251166
O	0	8.122356	0.290961	-1.214078
C	0	9.140757	1.140399	-1.734620
H	0	8.928210	2.201237	-1.543542
H	0	10.129540	0.893864	-1.324149
H	0	9.162098	0.978711	-2.815005
H	0	0.939542	1.784255	2.385019
O	0	0.097461	2.231487	2.173526
C	0	0.181701	3.577373	2.656270
H	0	0.253189	3.596423	3.750328
H	0	1.040644	4.101363	2.221356
H	0	-0.732451	4.088552	2.346327
Na	0	-1.211084	1.640133	0.368977
Na	0	-3.883669	-0.151619	-1.332150

Transition State, TS(**6** → **17**) shown in Figure S2-3
E=-2159.53880471 a.u. and thermal correction=0.531305 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=338.8489i cm^{-1}
SCRF=(PCM, solvent=methanol)= -2160.1492157 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-1.916283	-0.986774	-1.006503
O	0	-0.667536	-0.467995	-1.313199
C	0	-3.052809	-0.222568	-1.318592
C	0	-1.773958	-2.264721	-0.470640
C	0	-4.357420	-0.496146	-0.985281
C	0	-2.843800	-3.135947	-0.089331
C	0	-4.852550	-1.553000	-0.127145
C	0	-4.166235	-2.837033	0.023897
H	0	-2.862816	0.674426	-1.904292
H	0	-5.115490	0.191891	-1.352293
H	0	-2.554808	-4.164385	0.119792
H	0	-5.929281	-1.679721	-0.223467
H	0	-4.816620	-3.663064	0.307651
C	0	-0.372089	-2.544092	-0.457021
C	0	0.309959	-1.399462	-0.972537
N	0	1.577415	-1.151173	-1.125348
C	0	0.284484	-3.686967	0.005295
N	0	0.880227	-4.620582	0.391393
H	0	1.731028	-0.212301	-1.510435
O	0	3.405145	1.940218	1.123707
C	0	3.695586	2.579298	2.368745
H	0	3.223526	3.568601	2.416428
H	0	3.299414	1.954734	3.175456
H	0	4.777946	2.696567	2.514140

H	0	2.577853	-4.329653	1.278282
O	0	3.389286	-3.824118	1.499777
C	0	3.784121	-4.101208	2.843621
H	0	2.988865	-3.846300	3.555307
H	0	4.056707	-5.156456	2.965620
H	0	4.659561	-3.482301	3.054589
H	0	2.729025	-2.384485	-2.141654
O	0	3.584296	-2.874572	-2.139745
C	0	3.436526	-4.142096	-2.779762
H	0	2.668991	-4.754796	-2.289766
H	0	3.186661	-4.023695	-3.841759
H	0	4.399323	-4.652779	-2.701593
H	0	2.647107	2.438027	-1.663931
O	0	1.866531	1.814326	-1.858084
C	0	1.227934	2.202570	-3.070531
H	0	0.882534	3.245258	-3.026804
H	0	1.902382	2.090229	-3.929493
H	0	0.362074	1.550431	-3.216209
H	0	2.353843	4.296164	-0.231110
O	0	1.472767	4.428059	0.242569
C	0	0.785747	5.549323	-0.294609
H	0	1.329952	6.484103	-0.103227
H	0	0.626145	5.450641	-1.378047
H	0	-0.191056	5.610637	0.194897
H	0	3.646179	2.586884	0.322244
O	0	3.612690	3.443684	-0.865288
C	0	4.824294	3.937131	-1.381813
H	0	5.510953	3.120656	-1.664592
H	0	4.656158	4.547703	-2.283322
H	0	5.351858	4.572128	-0.650609
H	0	4.287392	0.494063	0.898746
O	0	4.796627	-0.349713	0.753937
C	0	6.157754	-0.028637	0.474383
H	0	6.243379	0.636110	-0.394728
H	0	6.640356	0.445502	1.338954
H	0	6.681039	-0.963345	0.253099
C	0	-5.048690	-0.845650	1.760660
H	0	-5.225929	-1.774908	2.302692
C	0	-3.826218	-0.202914	2.132468
N	0	-2.809734	0.316359	2.364094
C	0	-6.191779	0.015096	1.727316
N	0	-7.138110	0.680964	1.575938
H	0	-1.214526	1.315020	2.046615
O	0	-0.491959	1.964473	1.910205
C	0	-0.711330	3.064214	2.800958
H	0	-1.700862	3.509187	2.640975
H	0	-0.623531	2.746589	3.847132
H	0	0.055091	3.812291	2.583904
H	0	-7.439731	1.175139	-0.414727
O	0	-7.300974	1.190179	-1.379920
C	0	-8.391407	1.863781	-1.999213
H	0	-9.347671	1.357207	-1.808963
H	0	-8.469353	2.908418	-1.667809
H	0	-8.200506	1.853287	-3.075294
Na	0	3.527115	-2.070289	0.042602
Na	0	1.136726	2.113546	0.349869

The anion adduct 17 shown in Figure S2-4
E=-2159.53805264 a.u. and thermal correction=0.530725 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.153778 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-1.231150	-0.380664	-1.468655
O	0	0.143269	-0.095634	-1.514035
C	0	-2.145401	0.587300	-1.965183
C	0	-1.415496	-1.708593	-1.121697
C	0	-3.486953	0.563654	-1.748060
C	0	-2.685018	-2.395021	-1.140913
C	0	-4.172441	-0.360693	-0.774421
C	0	-3.907678	-1.819742	-1.071209

H	0	-1.729783	1.370778	-2.597213
H	0	-4.113098	1.275199	-2.277516
H	0	-2.638975	-3.475603	-1.261243
H	0	-5.250991	-0.193181	-0.817686
H	0	-4.789909	-2.442576	-1.190429
C	0	-0.104216	-2.277663	-0.949086
C	0	0.860271	-1.262491	-1.198026
N	0	2.160397	-1.266088	-1.134793
C	0	0.241174	-3.574103	-0.562456
N	0	0.588191	-4.639468	-0.213188
H	0	2.573744	-0.373003	-1.419832
O	0	2.509239	1.609200	1.462368
C	0	1.952062	2.089708	2.686825
H	0	1.338289	2.983117	2.513530
H	0	1.322190	1.302012	3.113073
H	0	2.737698	2.337911	3.412748
H	0	1.896050	-4.540269	1.227297
O	0	2.593561	-4.138518	1.790177
C	0	2.423885	-4.562123	3.143359
H	0	1.434554	-4.285296	3.528305
H	0	2.560113	-5.646084	3.237851
H	0	3.188897	-4.055931	3.737230
H	0	3.398238	-2.667215	-1.687645
O	0	4.158266	-3.223920	-1.395471
C	0	4.156194	-4.477636	-2.078414
H	0	3.212808	-5.017237	-1.927534
H	0	4.332067	-4.343008	-3.153257
H	0	4.974248	-5.070248	-1.661717
H	0	3.562121	2.338855	-1.168234
O	0	3.177437	1.642630	-1.803001
C	0	3.484941	1.982371	-3.151211
H	0	3.111965	2.983190	-3.409125
H	0	4.567010	1.947776	-3.332322
H	0	3.000577	1.248024	-3.801983
H	0	2.108230	4.065223	-0.204343
O	0	1.120939	4.008916	-0.370974
C	0	0.510488	5.298964	-0.338283
H	0	0.783096	5.839912	0.577293
H	0	0.810733	5.899092	-1.207978
H	0	-0.573291	5.164308	-0.348989
H	0	3.082753	2.380174	0.999263
O	0	3.627063	3.356384	0.082400
C	0	4.824033	4.008672	0.431481
H	0	5.651337	3.294087	0.584432
H	0	5.139917	4.709863	-0.356923
H	0	4.716070	4.590004	1.362252
H	0	3.530377	0.235346	1.686132
O	0	4.113383	-0.558534	1.832012
C	0	5.358393	-0.124606	2.375399
H	0	5.861499	0.585793	1.707116
H	0	5.222881	0.341634	3.359838
H	0	5.994861	-1.006442	2.493145
C	0	-3.732759	-0.023044	0.725265
H	0	-2.663761	-0.262259	0.805204
C	0	-3.902288	1.404538	1.026078
N	0	-4.025520	2.541894	1.216067
C	0	-4.474708	-0.849793	1.684556
N	0	-5.099767	-1.531738	2.385956
H	0	-3.371107	4.436101	0.686706
O	0	-3.005684	5.274152	0.351550
C	0	-3.915924	6.322700	0.662632
H	0	-4.894422	6.174134	0.184550
H	0	-4.063264	6.432129	1.746270
H	0	-3.478923	7.247388	0.276777
H	0	-6.643048	-2.380276	0.990422
O	0	-7.018311	-2.442739	0.095733
C	0	-8.349409	-2.947346	0.179901
H	0	-8.376738	-3.957501	0.609897
H	0	-9.000301	-2.287914	0.769578
H	0	-8.732260	-2.992479	-0.842256
Na	0	3.462793	-2.363706	0.641146

Na	0	1.242948	1.787381	-0.555176

Transition State, TS(**6** → **18**) shown in Figure S2-5
E=-2159.50903218 a.u. and thermal correction=0.527009 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=295.9425i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.1354485 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-1.794646	-0.651672	-0.617691
O	0	-0.478731	-0.231852	-0.538898
C	0	-2.764135	0.289029	-0.726626
C	0	-1.836301	-2.102042	-0.541030
C	0	-4.196591	0.067349	-0.673458
C	0	-2.965263	-2.886480	-0.706846
C	0	-4.812996	-1.178817	-1.066829
C	0	-4.275189	-2.444808	-1.018793
H	0	-2.425227	1.320736	-0.762135
H	0	-4.765534	0.940911	-0.981550
H	0	-2.814091	-3.962893	-0.674278
H	0	-5.855697	-1.105417	-1.366864
H	0	-4.966058	-3.245547	-1.277790
C	0	-0.476995	-2.499216	-0.349433
C	0	0.347308	-1.333774	-0.344020
N	0	1.624489	-1.199707	-0.189040
C	0	0.044065	-3.776421	-0.131078
N	0	0.546667	-4.815704	0.076562
H	0	1.901136	-0.213459	-0.132250
O	0	2.906315	1.354682	0.940564
C	0	2.008887	1.986192	1.858278
H	0	1.177414	2.473295	1.337009
H	0	1.599436	1.212019	2.513875
H	0	2.527300	2.732175	2.474991
H	0	2.041800	-4.862587	1.300126
O	0	2.821520	-4.537611	1.802004
C	0	3.051470	-5.380056	2.932527
H	0	2.189316	-5.381431	3.610302
H	0	3.271837	-6.407894	2.620853
H	0	3.918292	-4.978144	3.463100
H	0	2.865109	-2.216652	-1.323630
O	0	3.705350	-2.730768	-1.353257
C	0	3.574471	-3.848209	-2.235558
H	0	2.742496	-4.499443	-1.940943
H	0	3.431062	-3.519544	-3.272804
H	0	4.507667	-4.413040	-2.172946
H	0	4.292816	1.884943	-1.945359
O	0	4.194883	1.492398	-2.863376
C	0	5.025254	0.349356	-3.061047
H	0	6.086229	0.612635	-2.964040
H	0	4.780762	-0.453234	-2.355357
H	0	4.847777	-0.009376	-4.078422
H	0	2.252153	4.107602	-0.877792
O	0	1.522263	4.402951	-1.483753
C	0	0.585127	5.268185	-0.829935
H	0	0.159730	4.802291	0.064798
H	0	1.060139	6.220488	-0.562540
H	0	-0.216673	5.466985	-1.545460
H	0	3.263938	2.047266	0.276847
O	0	3.748397	3.066273	-0.808777
C	0	4.841603	3.845471	-0.372325
H	0	5.224992	3.502730	0.603565
H	0	5.685208	3.804656	-1.083480
H	0	4.569496	4.908757	-0.257457
H	0	3.884821	0.117201	1.566429
O	0	4.356989	-0.700001	1.889340
C	0	5.504300	-0.321565	2.643462
H	0	6.205432	0.267278	2.037995
H	0	5.225239	0.257738	3.532870
H	0	6.006806	-1.237530	2.967399
C	0	-4.672560	0.324555	1.327524
H	0	-4.239404	-0.599701	1.707785
C	0	-3.984759	1.494002	1.765408

N	0	-3.343028	2.434218	2.020771
C	0	-6.097036	0.355204	1.377811
N	0	-7.261635	0.332499	1.300034
H	0	-1.784212	3.662781	2.073475
O	0	-1.009292	4.258117	2.102315
C	0	-1.164795	5.135079	3.211072
H	0	-2.075073	5.745325	3.128331
H	0	-1.191483	4.590193	4.165225
H	0	-0.298778	5.803188	3.217740
H	0	-8.099491	-0.273381	-0.452038
O	0	-8.204567	-0.600014	-1.366028
C	0	-9.566526	-0.467537	-1.753842
H	0	-10.234547	-1.066007	-1.118713
H	0	-9.900146	0.579427	-1.732487
H	0	-9.642312	-0.835022	-2.780618
Na	0	3.352100	-2.485838	0.958161
Na	0	2.563507	2.978946	-2.789847

The anion adduct **18** shown in Figure S2-6
E=-2159.53669857 a.u. and thermal correction=0.534161 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.152006 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-1.411018	-1.068807	-0.986011
O	0	-0.126800	-0.639749	-1.335736
C	0	-2.466327	-0.258547	-1.198127
C	0	-1.316323	-2.389084	-0.377339
C	0	-3.832311	-0.517445	-0.624346
C	0	-2.373582	-3.246856	-0.170175
C	0	-4.368422	-1.892916	-0.926347
C	0	-3.725315	-3.047852	-0.615653
H	0	-2.309534	0.666775	-1.747425
H	0	-4.524839	0.229414	-1.020023
H	0	-2.128551	-4.238263	0.203947
H	0	-5.370695	-1.934801	-1.342794
H	0	-4.294558	-3.966863	-0.751425
C	0	0.098472	-2.630413	-0.238389
C	0	0.819024	-1.581666	-0.867085
N	0	2.086342	-1.382950	-1.032666
C	0	0.734460	-3.730052	0.339441
N	0	1.317531	-4.614228	0.845302
H	0	2.293018	-0.536818	-1.575255
O	0	2.269495	2.058211	0.791204
C	0	1.873236	2.733427	1.993783
H	0	1.083225	3.467571	1.801459
H	0	1.493651	1.982968	2.693964
H	0	2.728914	3.242004	2.457146
H	0	2.776908	-3.997567	1.978538
O	0	3.471951	-3.383224	2.301092
C	0	3.596698	-3.496298	3.719186
H	0	2.649157	-3.269654	4.223557
H	0	3.930992	-4.500115	4.007348
H	0	4.348139	-2.768489	4.034963
H	0	3.494934	-2.717781	-1.506235
O	0	4.372365	-3.055939	-1.218458
C	0	4.512316	-4.437262	-1.556315
H	0	3.711760	-5.042280	-1.113186
H	0	4.520110	-4.578863	-2.644275
H	0	5.472542	-4.767205	-1.152917
H	0	2.847144	2.189770	-2.074073
O	0	2.504001	1.309124	-2.455434
C	0	2.423097	1.395339	-3.876014
H	0	1.816097	2.255196	-4.189580
H	0	3.421140	1.477592	-4.325426
H	0	1.951252	0.478201	-4.242117
H	0	1.288365	3.882375	-1.486550
O	0	0.310541	3.673620	-1.608834
C	0	-0.489558	4.826106	-1.351186
H	0	-0.437637	5.128292	-0.298225
H	0	-0.187030	5.664414	-1.992466

H	0	-1.525877	4.568069	-1.588999
H	0	2.630391	2.754418	0.085859
O	0	2.884691	3.510152	-1.156094
C	0	3.970407	4.403226	-1.209180
H	0	4.925859	3.900258	-0.979700
H	0	4.071023	4.852064	-2.210351
H	0	3.853400	5.230107	-0.489321
H	0	3.541915	0.933461	1.089233
O	0	4.280206	0.292301	1.280861
C	0	5.491283	1.024883	1.458271
H	0	5.737417	1.613387	0.565378
H	0	5.427636	1.695227	2.324954
H	0	6.293864	0.302854	1.635198
C	0	-3.812635	-0.303655	0.968324
H	0	-3.179746	-1.101078	1.381119
C	0	-3.228141	0.990922	1.341154
N	0	-2.743598	2.016318	1.583764
C	0	-5.165002	-0.439665	1.521998
N	0	-6.259078	-0.555683	1.891863
H	0	-1.723497	3.750747	2.043878
O	0	-1.185280	4.537177	2.244337
C	0	-1.947047	5.415358	3.065384
H	0	-2.856583	5.767357	2.558468
H	0	-2.230758	4.946002	4.017822
H	0	-1.313389	6.279621	3.280226
H	0	-7.531547	-0.902868	0.125201
O	0	-7.687048	-0.986782	-0.830936
C	0	-9.077891	-0.822196	-1.094556
H	0	-9.682321	-1.595780	-0.601771
H	0	-9.439827	0.167405	-0.783926
H	0	-9.205365	-0.916281	-2.175546
Na	0	3.820391	-1.825511	0.665039
Na	0	0.746792	1.560652	-0.958806

Transition State, TS(**6** → **7**) shown in Figure S2-7
E=-2159.51284201 a.u. and thermal correction=0.529544 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=305.0464i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.137998 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-0.326645	2.764510	-0.754874
O	0	0.224666	1.500514	-0.592021
C	0	0.553911	3.704139	-1.386469
C	0	-1.742094	2.593425	-1.132063
C	0	0.210875	4.979614	-1.771614
C	0	-2.620236	3.622667	-1.458196
C	0	-1.063884	5.593177	-1.779877
C	0	-2.305280	4.977807	-1.650481
H	0	1.592687	3.394496	-1.449629
H	0	1.034915	5.604844	-2.110623
H	0	-3.666176	3.344551	-1.565185
H	0	-1.077281	6.656592	-2.004785
H	0	-3.165693	5.630257	-1.789883
C	0	-1.996272	1.208127	-1.005173
C	0	-0.782090	0.537681	-0.638722
N	0	-0.539202	-0.703255	-0.396532
C	0	-3.218752	0.552219	-1.208309
N	0	-4.237763	0.002922	-1.373474
H	0	0.441268	-0.856294	-0.130066
O	0	2.049939	-1.517266	1.090359
C	0	2.674031	-0.430386	1.779473
H	0	3.215517	0.223718	1.087080
H	0	1.889129	0.155590	2.265734
H	0	3.372118	-0.792233	2.546190
H	0	-5.608852	-1.300125	-0.744269
O	0	-6.208373	-1.989603	-0.398453
C	0	-7.503546	-1.775884	-0.942048
H	0	-7.921293	-0.802612	-0.645757
H	0	-7.507333	-1.839976	-2.039832
H	0	-8.151143	-2.563894	-0.547816

H	0	-1.527082	-2.293399	-1.051466
O	0	-1.983105	-3.113732	-0.754648
C	0	-2.959201	-3.535721	-1.710800
H	0	-3.680170	-2.740457	-1.927124
H	0	-2.479526	-3.863910	-2.642317
H	0	-3.492354	-4.380759	-1.270135
H	0	2.631689	-3.801503	-1.114897
O	0	2.228409	-4.070554	-1.990782
C	0	1.091044	-4.918314	-1.828510
H	0	1.370538	-5.859258	-1.338099
H	0	0.300080	-4.424634	-1.252284
H	0	0.712179	-5.146278	-2.828382
H	0	4.683060	-1.364986	-0.940765
O	0	4.907184	-0.865007	-1.772649
C	0	5.665810	0.320637	-1.509251
H	0	5.173667	0.959865	-0.768904
H	0	6.675023	0.065616	-1.161653
H	0	5.748306	0.864279	-2.453902
H	0	2.755297	-2.037702	0.564057
O	0	3.813338	-2.804717	-0.308219
C	0	4.676259	-3.602064	0.473921
H	0	4.494629	-3.465267	1.553185
H	0	4.550707	-4.677533	0.259042
H	0	5.737293	-3.358732	0.291332
H	0	0.855983	-2.377565	1.959127
O	0	0.048384	-2.770888	2.386955
C	0	0.395131	-3.344479	3.643177
H	0	1.121307	-4.158956	3.522817
H	0	0.808464	-2.593089	4.328744
H	0	-0.518353	-3.752844	4.084207
H	0	-0.941767	4.390689	1.011534
C	0	-0.462099	3.434168	1.218974
C	0	0.904104	3.549453	1.612821
N	0	2.048108	3.627115	1.824985
C	0	-1.256892	2.551134	2.008810
N	0	-1.924072	1.803538	2.606908
H	0	-2.805266	0.098067	2.693499
O	0	-3.196544	-0.783586	2.513359
C	0	-4.625683	-0.669557	2.543164
H	0	-4.981668	-0.539020	3.572556
H	0	-4.965097	0.171047	1.927962
H	0	-5.042105	-1.587857	2.124955
H	0	3.840097	2.981180	1.251541
O	0	4.711205	2.648493	0.958054
C	0	5.716703	3.298977	1.725360
H	0	5.707830	4.387776	1.575681
H	0	5.614444	3.089587	2.799376
H	0	6.681476	2.910554	1.386884
Na	0	-1.790780	-2.065089	1.294659
Na	0	3.625506	-2.462118	-2.575792

The anion adduct **7** shown in Figure S2-8
E=-2159.51935220 a.u. and thermal correction=0.524803 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.141145 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-0.611146	0.537284	-1.340984
O	0	0.750032	1.064828	-1.331166
C	0	-1.219143	0.830528	-2.679104
C	0	-0.442163	-0.955702	-1.092069
C	0	-2.396830	0.321751	-3.115749
C	0	-1.460379	-1.874473	-1.122578
C	0	-3.204753	-0.704531	-2.516321
C	0	-2.776537	-1.678559	-1.652279
H	0	-0.672135	1.549075	-3.282742
C	0	-1.381559	1.275496	-0.172519
H	0	-2.465009	0.910733	-0.091576
H	0	-4.234650	-0.768281	-2.855179
H	0	-3.501810	-2.453447	-1.407555
C	0	0.951719	-1.143924	-0.815681

C	0	1.636511	0.090055	-0.976004
N	0	2.916967	0.345464	-0.861045
C	0	1.651523	-2.337625	-0.640962
N	0	2.309470	-3.301727	-0.506217
H	0	3.097622	1.314839	-1.129420
O	0	-3.992113	0.497806	0.691351
C	0	-4.328682	1.599595	1.492627
H	0	-3.443539	2.215096	1.744931
H	0	-5.044833	2.277947	0.996011
H	0	-4.781756	1.303036	2.458574
H	0	3.803381	-3.762038	-1.724576
O	0	4.601911	-3.376676	-2.144183
C	0	5.328672	-4.373575	-2.865161
H	0	5.670307	-5.175327	-2.199823
H	0	4.719385	-4.799397	-3.670702
H	0	6.199339	-3.880411	-3.303224
H	0	3.542048	0.488441	0.897203
O	0	4.093592	0.572856	1.718471
C	0	3.335601	0.175837	2.871368
H	0	2.407017	0.750362	2.945878
H	0	3.099453	-0.894433	2.834480
H	0	3.959355	0.375094	3.745526
H	0	5.331755	2.005943	1.700599
O	0	6.165851	2.504002	1.594422
C	0	5.919721	3.890337	1.802102
H	0	5.197022	4.294519	1.079289
H	0	5.556153	4.096436	2.818751
H	0	6.872219	4.408245	1.664475
H	0	-5.685576	-2.063160	0.334604
O	0	-5.214540	-2.767103	0.869829
C	0	-5.906985	-4.007244	0.790347
H	0	-6.918341	-3.928911	1.209915
H	0	-5.976822	-4.362780	-0.246079
H	0	-5.343765	-4.740467	1.374498
H	0	-5.230399	-0.075370	-0.083154
O	0	-6.009992	-0.621699	-0.481048
C	0	-7.234173	0.075670	-0.293886
H	0	-7.435792	0.276294	0.768554
H	0	-7.231564	1.030432	-0.836166
H	0	-8.044200	-0.544281	-0.691203
H	0	5.576770	-0.318768	1.109116
O	0	6.105644	-0.837455	0.461924
C	0	7.500136	-0.553084	0.639360
H	0	7.872510	-1.005803	1.565940
H	0	8.029600	-0.997530	-0.207453
H	0	7.674613	0.527003	0.661284
H	0	-1.219585	-2.880780	-0.780420
H	0	-2.776511	0.731164	-4.051081
C	0	-1.414004	2.721242	-0.407969
N	0	-1.453612	3.859991	-0.623537
C	0	-0.799447	0.972492	1.138209
N	0	-0.386861	0.646956	2.174585
H	0	-1.256265	-0.966452	3.018253
O	0	-1.883056	-1.714644	3.076575
C	0	-1.508255	-2.579755	4.151854
H	0	-0.515125	-3.013017	3.984205
H	0	-1.520808	-2.047391	5.110039
H	0	-2.245561	-3.385204	4.185148
H	0	-0.992913	5.816274	-1.130044
O	0	-0.820212	6.751539	-1.340204
C	0	-1.936423	7.517695	-0.911736
H	0	-2.864052	7.221633	-1.423302
H	0	-2.096250	7.446906	0.174284
H	0	-1.722507	8.560607	-1.161501
Na	0	-3.437760	-1.496539	1.423277
Na	0	4.557043	-1.392217	-1.061261

Transition State, TS(**7** → **7a**) shown in Figure S2-9
E=-2159.51754608 a.u. and thermal correction=0.523280 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=744.7065i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.140266 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-0.649457	0.510755	-1.294669
O	0	0.720126	1.051878	-1.345885
C	0	-1.280859	0.778173	-2.629389
C	0	-0.441260	-0.979622	-1.038557
C	0	-2.427910	0.215798	-3.079273
C	0	-1.427342	-1.935757	-1.064978
C	0	-3.193833	-0.855262	-2.502543
C	0	-2.739145	-1.806392	-1.627363
H	0	-0.773295	1.529295	-3.227937
C	0	-1.379646	1.256557	-0.123324
H	0	-2.584887	0.842910	0.063876
H	0	-4.208313	-0.973570	-2.872323
H	0	-3.428238	-2.620714	-1.404451
C	0	0.956912	-1.138113	-0.776906
C	0	1.621028	0.102412	-0.982385
N	0	2.902874	0.369618	-0.897912
C	0	1.678035	-2.318184	-0.596033
N	0	2.352334	-3.270628	-0.458419
H	0	3.069399	1.334094	-1.191779
O	0	-3.815758	0.475443	0.583880
C	0	-4.228238	1.507744	1.459809
H	0	-3.368130	2.077439	1.849482
H	0	-4.892591	2.229303	0.959723
H	0	-4.765473	1.101787	2.332997
H	0	3.826649	-3.744507	-1.693364
O	0	4.613960	-3.360590	-2.135063
C	0	5.337156	-4.364961	-2.848759
H	0	5.700471	-5.148752	-2.173508
H	0	4.717067	-4.814471	-3.632962
H	0	6.193723	-3.872318	-3.314377
H	0	3.544145	0.548356	0.846019
O	0	4.100217	0.648885	1.663216
C	0	3.358703	0.239722	2.823528
H	0	2.404764	0.772211	2.885641
H	0	3.171431	-0.840709	2.805793
H	0	3.971848	0.482559	3.694268
H	0	5.315955	2.091325	1.635043
O	0	6.138948	2.608040	1.527822
C	0	5.868659	3.983986	1.766968
H	0	5.129581	4.388853	1.060946
H	0	5.512954	4.162621	2.791693
H	0	6.809084	4.523667	1.629245
H	0	-5.631440	-2.084878	0.414428
O	0	-5.147401	-2.747411	0.980056
C	0	-5.859214	-3.979842	1.028481
H	0	-6.850060	-3.850971	1.482256
H	0	-5.976373	-4.414971	0.027587
H	0	-5.280039	-4.671584	1.646153
H	0	-5.150545	-0.139297	-0.219756
O	0	-5.948875	-0.676927	-0.521017
C	0	-7.131122	0.110349	-0.412754
H	0	-7.318280	0.429306	0.622042
H	0	-7.071422	0.999586	-1.052682
H	0	-7.971369	-0.504063	-0.748322
H	0	5.581817	-0.232339	1.050225
O	0	6.113737	-0.752778	0.406307
C	0	7.505625	-0.452963	0.575048
H	0	7.886276	-0.890970	1.505390
H	0	8.036530	-0.901730	-0.268604
H	0	7.670185	0.628964	0.583852
H	0	-1.145077	-2.932206	-0.723873
H	0	-2.817631	0.615817	-4.014553
C	0	-1.502168	2.679625	-0.389785
N	0	-1.657812	3.806188	-0.629191
C	0	-0.762737	0.995289	1.163740
N	0	-0.345199	0.679145	2.205170
H	0	-1.212532	-0.897974	3.021250
O	0	-1.831000	-1.655055	3.090030
C	0	-1.512779	-2.440475	4.241012

H	0	-0.506148	-2.868131	4.162871
H	0	-1.588928	-1.845721	5.158757
H	0	-2.241104	-3.253718	4.285536
H	0	-2.164250	5.715916	-1.185011
O	0	-2.320932	6.650524	-1.414152
C	0	-1.240485	7.418175	-0.907668
H	0	-1.160659	7.351867	0.187674
H	0	-0.276850	7.120584	-1.347480
H	0	-1.434252	8.460580	-1.176170
Na	0	-3.259573	-1.560327	1.324327
Na	0	4.552929	-1.357115	-1.086134

The di-anion **7a** shown in Figure S2-10
E=-2159.56180052 a.u. and thermal correction=0.539706 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.181473 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	0.563459	-2.007811	-0.616907
O	0	-0.518318	-2.888232	-0.092294
C	0	1.250112	-2.784441	-1.708362
C	0	-0.206907	-0.824996	-1.193958
C	0	2.158823	-2.259924	-2.564654
C	0	0.384861	0.204334	-1.887209
C	0	2.502195	-0.872131	-2.743484
C	0	1.693397	0.206855	-2.453198
H	0	1.003289	-3.841244	-1.751467
C	0	1.484485	-1.618185	0.523839
N	0	0.807776	0.261379	2.147332
H	0	3.409406	-0.664561	-3.310105
H	0	2.054554	1.175083	-2.798277
C	0	-1.570045	-0.996651	-0.807419
C	0	-1.716592	-2.251523	-0.122429
N	0	-2.779128	-2.797056	0.390981
C	0	-2.615935	-0.153228	-1.159333
N	0	-3.472539	0.594622	-1.459366
H	0	-2.543496	-3.715394	0.769005
O	0	2.320477	2.513712	2.364770
C	0	2.146203	3.230920	3.591068
H	0	2.253767	2.562527	4.452976
H	0	2.921651	3.999483	3.632729
H	0	1.161638	3.711621	3.628125
H	0	-4.535388	2.225864	-2.137240
O	0	-5.269536	2.761629	-1.776372
C	0	-5.673527	3.774431	-2.696785
H	0	-4.854311	4.473526	-2.903530
H	0	-6.028524	3.339239	-3.638856
H	0	-6.494471	4.321011	-2.227689
H	0	-4.073184	-2.120701	1.106268
O	0	-4.867521	-1.739819	1.643282
C	0	-5.193223	-2.637889	2.706247
H	0	-5.504005	-3.614485	2.314635
H	0	-4.337398	-2.775751	3.378179
H	0	-6.022213	-2.203233	3.271325
H	0	-6.120175	-1.138254	0.559044
O	0	-6.659254	-0.548659	-0.024892
C	0	-7.110448	-1.287736	-1.161555
H	0	-6.268941	-1.707298	-1.726618
H	0	-7.787892	-2.097026	-0.862243
H	0	-7.658744	-0.593658	-1.803940
H	0	3.804614	2.671795	-0.966736
O	0	4.429677	2.025816	-1.379476
C	0	5.750238	2.565101	-1.301475
H	0	5.816604	3.526201	-1.826362
H	0	6.068393	2.696441	-0.259445
H	0	6.422636	1.853932	-1.789740
H	0	3.773006	1.416040	2.019519
O	0	4.412006	0.760968	1.663081
C	0	4.954903	-0.007041	2.742480
H	0	5.499360	0.636147	3.446006
H	0	4.170279	-0.555980	3.276507

H	0	5.650631	-0.724560	2.303984
H	0	-4.485514	-0.043757	2.059199
O	0	-4.408295	0.940681	2.021610
C	0	-3.127477	1.334915	2.529483
H	0	-3.039199	1.096976	3.596157
H	0	-2.309474	0.852832	1.982164
H	0	-3.051068	2.418445	2.405411
H	0	-0.222250	1.089146	-2.072185
H	0	2.671124	-2.961883	-3.222444
C	0	2.566813	-2.439256	0.860260
N	0	3.520360	-3.091501	1.088932
C	0	1.114202	-0.610350	1.416312
H	0	1.657974	1.763872	2.314324
H	0	2.504550	3.353141	0.791220
O	0	2.683531	3.729131	-0.102773
C	0	1.444890	4.063527	-0.730553
H	0	0.799289	3.183236	-0.842858
H	0	0.910578	4.835459	-0.162451
H	0	1.682642	4.460257	-1.720665
H	0	4.994345	-2.415620	0.148006
O	0	5.527356	-1.775622	-0.384827
C	0	6.401121	-2.488620	-1.256211
H	0	7.108587	-3.106305	-0.689432
H	0	5.842972	-3.128310	-1.952305
H	0	6.964503	-1.747782	-1.830126
Na	0	3.984681	-0.060953	-0.455259
Na	0	-5.326109	1.301207	-0.034654

Transition State, TS(**7a** → **8**) shown in Figure S2-11
E=-2159.54221154 a.u. and thermal correction=0.532542 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=877.6168i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.172611 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-0.049744	-2.642372	0.044789
O	0	-1.092641	-2.627151	1.138481
C	0	0.011692	-4.066986	-0.435132
C	0	-0.663407	-1.725299	-1.004640
C	0	0.664770	-4.453745	-1.554464
C	0	-0.143671	-1.541401	-2.251625
C	0	1.254116	-3.611545	-2.565626
C	0	0.882333	-2.330325	-2.870624
H	0	-0.464284	-4.802782	0.206782
C	0	1.246987	-2.119930	0.592590
N	0	1.938852	0.348548	0.520066
H	0	1.983545	-4.086545	-3.218557
H	0	1.342380	-1.886669	-3.752939
C	0	-1.785792	-1.070182	-0.369477
C	0	-2.003840	-1.668194	0.905924
N	0	-2.933215	-1.433495	1.803039
C	0	-2.499799	-0.006909	-0.890035
N	0	-3.061368	0.923464	-1.350484
H	0	-2.820152	-2.018697	2.627238
O	0	2.136352	3.054796	0.985122
C	0	1.028775	3.817234	1.497368
H	0	0.750039	3.466588	2.498107
H	0	1.361816	4.855559	1.563945
H	0	0.164632	3.749840	0.827931
H	0	-2.170704	2.699026	-0.896309
O	0	-1.823250	3.594757	-0.711562
C	0	-2.056116	4.411098	-1.850540
H	0	-1.544752	4.029501	-2.746012
H	0	-3.128846	4.511945	-2.076160
H	0	-1.660887	5.404292	-1.621257
H	0	-4.073263	-0.874430	1.670691
O	0	-5.216965	-0.443485	1.617646
C	0	-5.953009	-0.918537	2.736153
H	0	-5.963620	-2.018387	2.770714
H	0	-5.527435	-0.548512	3.680832
H	0	-6.992092	-0.571701	2.672602
H	0	-5.902394	-0.858458	0.146923

O	0	-6.213442	-0.839156	-0.807959
C	0	-6.005802	-2.115372	-1.411323
H	0	-4.951268	-2.416765	-1.363515
H	0	-6.622183	-2.884355	-0.929424
H	0	-6.303901	-2.039035	-2.460703
H	0	4.321316	2.148581	-1.591336
O	0	4.996371	1.436154	-1.445172
C	0	6.216746	1.799822	-2.085267
H	0	6.076120	1.925361	-3.166180
H	0	6.630836	2.725999	-1.666008
H	0	6.929944	0.987261	-1.920740
H	0	3.738189	2.559239	1.808819
O	0	4.510378	1.990832	2.026959
C	0	4.596715	1.837785	3.444987
H	0	4.788477	2.799931	3.936019
H	0	3.682547	1.392817	3.858773
H	0	5.436097	1.167872	3.646471
H	0	-5.436731	1.209441	1.350070
O	0	-5.621763	2.087391	0.903529
C	0	-4.991127	3.148945	1.620926
H	0	-5.349462	3.188707	2.657136
H	0	-3.899058	3.048159	1.614452
H	0	-5.258619	4.086005	1.125235
H	0	-0.562216	-0.734999	-2.852744
H	0	0.744939	-5.526737	-1.726386
C	0	2.223484	-2.937685	1.178675
N	0	3.121653	-3.528968	1.654786
C	0	1.574297	-0.774470	0.558529
H	0	1.874291	2.103615	0.878556
H	0	2.693474	3.345937	-0.723161
O	0	3.026626	3.307114	-1.650727
C	0	1.949752	2.905708	-2.505442
H	0	1.555093	1.923435	-2.218406
H	0	1.138947	3.643451	-2.483462
H	0	2.350846	2.850464	-3.520505
H	0	4.641862	-2.433023	1.221851
O	0	5.290182	-1.728238	0.990505
C	0	6.596389	-2.304475	0.942179
H	0	6.869038	-2.744609	1.908602
H	0	6.662328	-3.072409	0.162105
H	0	7.299526	-1.499993	0.708984
Na	0	4.415789	0.303612	0.429553
Na	0	-5.357892	1.202309	-1.133463

The mono-anion intermediate **8** shown in Figure S2-12
E=-2159.54583821 a.u. and thermal correction=0.532753 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.172057 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-0.061873	-2.686052	-0.038535
O	0	1.053884	-2.760771	-1.085128
C	0	-0.171499	-4.079767	0.513322
C	0	0.532960	-1.723996	0.980499
C	0	-0.868985	-4.389300	1.629574
C	0	-0.024779	-1.459474	2.194568
C	0	-1.474438	-3.481352	2.572352
C	0	-1.088986	-2.192438	2.819809
H	0	0.305192	-4.860584	-0.072131
C	0	-1.307084	-2.176394	-0.688537
N	0	-1.881404	0.315330	-0.907690
H	0	-2.234210	-3.907164	3.224424
H	0	-1.567415	-1.693092	3.661480
C	0	1.702530	-1.131573	0.362313
C	0	1.956473	-1.812643	-0.847358
N	0	2.935161	-1.664171	-1.729695
C	0	2.439004	-0.071147	0.872540
N	0	3.010392	0.852398	1.324930
H	0	2.911332	-2.291554	-2.524020
O	0	-2.083245	3.079210	-0.917122
C	0	-0.998329	3.907032	-1.373209

H	0	-0.746035	3.670725	-2.413347
H	0	-1.343585	4.941857	-1.315834
H	0	-0.119593	3.779520	-0.732552
H	0	1.982869	2.635468	1.169833
O	0	1.557258	3.514308	1.133763
C	0	2.499566	4.486566	1.566972
H	0	2.832068	4.306657	2.599663
H	0	3.380544	4.528001	0.908932
H	0	1.999077	5.457662	1.531332
H	0	3.829239	-1.096537	-1.587441
O	0	5.306394	-0.418371	-1.555108
C	0	6.047447	-0.858995	-2.671824
H	0	6.126630	-1.959720	-2.700805
H	0	5.584177	-0.537592	-3.620374
H	0	7.075732	-0.460682	-2.660859
H	0	6.040412	-0.735510	-0.196752
O	0	6.393598	-0.673876	0.764507
C	0	6.807104	-1.943551	1.244723
H	0	5.988686	-2.675976	1.209657
H	0	7.655458	-2.332519	0.665740
H	0	7.124285	-1.827735	2.285724
H	0	-4.164926	1.819647	1.618312
O	0	-4.817735	1.107865	1.389885
C	0	-5.476660	0.656398	2.570098
H	0	-4.765349	0.236319	3.293193
H	0	-6.037994	1.469623	3.047653
H	0	-6.177306	-0.129128	2.274697
H	0	-3.738532	2.781569	-1.652180
O	0	-4.591869	2.321551	-1.821709
C	0	-5.661202	3.265142	-1.740316
H	0	-5.716992	3.725476	-0.745731
H	0	-5.555784	4.048653	-2.500770
H	0	-6.589387	2.719797	-1.929659
H	0	5.364858	1.153880	-1.418755
O	0	5.419425	2.108990	-1.050872
C	0	4.779762	3.021319	-1.931045
H	0	5.302859	3.077758	-2.895212
H	0	3.731723	2.744907	-2.111770
H	0	4.802937	4.013845	-1.469857
H	0	0.396118	-0.634736	2.768258
H	0	-0.979473	-5.449071	1.856214
C	0	-2.296691	-3.015945	-1.221784
N	0	-3.202583	-3.621683	-1.662115
C	0	-1.573097	-0.819159	-0.811007
H	0	-1.827808	2.124351	-0.972989
H	0	-2.570271	3.130891	0.843110
O	0	-2.879449	2.999379	1.769234
C	0	-1.764988	2.549537	2.554087
H	0	-1.489948	1.518052	2.297763
H	0	-0.894450	3.197069	2.406574
H	0	-2.074319	2.591297	3.601644
H	0	-4.701250	-2.425600	-1.405151
O	0	-5.316651	-1.661608	-1.324141
C	0	-6.530826	-1.979788	-2.008191
H	0	-6.349608	-2.161792	-3.074131
H	0	-7.011897	-2.859728	-1.565482
H	0	-7.198935	-1.120623	-1.902283
Na	0	-4.372261	0.316622	-0.683571
Na	0	5.305405	1.228221	0.984034

Transition State, TS(**8** → **9**) shown in Figure S2-13
E=-2159.53679113 a.u. and thermal correction=0.532682 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=154.5352i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.160647 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	0.341140	2.843932	-0.075655
O	0	-1.011388	2.736303	-1.574261
C	0	0.394258	4.306575	0.085223
C	0	-0.551578	2.091420	0.859084
C	0	0.688535	4.914846	1.263550

C	0	-0.367886	2.150062	2.217563
C	0	0.881204	4.309713	2.552258
C	0	0.428014	3.080988	2.955456
H	0	0.292767	4.893934	-0.822134
C	0	1.453830	2.177079	-0.646256
N	0	1.846287	-0.368652	-0.595179
H	0	1.368651	4.930107	3.300695
H	0	0.588083	2.824952	4.001698
C	0	-1.528793	1.295389	0.151632
C	0	-1.766462	1.781433	-1.184963
N	0	-2.719147	1.293264	-2.002984
C	0	-2.258623	0.278750	0.749362
N	0	-2.840065	-0.607498	1.265935
H	0	-2.815506	1.784854	-2.882282
O	0	1.876025	-3.200878	-0.481015
C	0	0.766863	-4.065746	-0.803273
H	0	0.459493	-3.921704	-1.845448
H	0	1.123646	-5.089666	-0.673201
H	0	-0.074970	-3.879495	-0.129343
H	0	-1.966679	-2.391593	1.475272
O	0	-1.596983	-3.290010	1.601300
C	0	-2.577696	-4.089613	2.251224
H	0	-2.828501	-3.701260	3.248580
H	0	-3.499963	-4.171027	1.657596
H	0	-2.153150	-5.090468	2.366978
H	0	-3.546504	0.729471	-1.701707
O	0	-5.143616	-0.026474	-1.560750
C	0	-5.745411	0.267787	-2.800317
H	0	-5.794195	1.356006	-2.985505
H	0	-5.188216	-0.178311	-3.643532
H	0	-6.779459	-0.113672	-2.859755
H	0	-6.024958	0.735418	-0.394124
O	0	-6.417670	0.861247	0.531390
C	0	-6.547907	2.237642	0.857981
H	0	-5.590257	2.770312	0.772875
H	0	-7.286936	2.732796	0.213977
H	0	-6.892797	2.304111	1.894009
H	0	4.063034	-1.880448	1.908356
O	0	4.750464	-1.231099	1.602527
C	0	5.761203	-1.093963	2.598505
H	0	5.343640	-0.714990	3.539770
H	0	6.267757	-2.048935	2.787049
H	0	6.494146	-0.372154	2.227777
H	0	3.467338	-3.018365	-1.386559
O	0	4.280251	-2.574557	-1.719845
C	0	4.503223	-2.937342	-3.083084
H	0	4.674448	-4.016127	-3.181907
H	0	3.660985	-2.641378	-3.721543
H	0	5.399842	-2.408985	-3.416026
H	0	-5.172217	-1.658795	-1.402011
O	0	-5.226090	-2.548056	-0.916630
C	0	-4.420482	-3.526950	-1.556197
H	0	-4.796155	-3.758713	-2.562227
H	0	-3.371849	-3.206621	-1.633230
H	0	-4.461432	-4.440283	-0.955031
H	0	-0.929672	1.430695	2.812078
H	0	0.830204	5.993765	1.220777
C	0	2.519387	2.853309	-1.287166
N	0	3.471469	3.305224	-1.796245
C	0	1.608192	0.778744	-0.619068
H	0	1.611281	-2.258264	-0.574146
H	0	2.402971	-3.153014	1.292221
O	0	2.742051	-2.956328	2.194242
C	0	1.676787	-2.384053	2.970699
H	0	1.478907	-1.347677	2.667949
H	0	0.757425	-2.967969	2.864306
H	0	2.000885	-2.398105	4.014186
H	0	4.917469	1.996334	-1.580340
O	0	5.452119	1.190814	-1.411958
C	0	6.801245	1.435763	-1.821720
H	0	6.853682	1.655490	-2.894324

H	0	7.239955	2.266283	-1.256802
H	0	7.371744	0.526151	-1.616520
Na	0	4.386567	-0.623979	-0.526536
Na	0	-5.095686	-0.956140	0.692159

The anion **9** shown in Figure S2-14
E=-2159.55283159 a.u. and thermal correction=0.533749 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.176691a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	0.433608	3.262168	0.570518
O	0	-0.041175	1.779373	-1.827838
C	0	0.557247	4.671333	0.464410
C	0	-0.851704	2.608583	0.872702
C	0	-0.183602	5.688378	1.050742
C	0	-1.674035	3.115658	1.902873
C	0	-1.198070	5.583258	2.006356
C	0	-1.794580	4.399904	2.434894
H	0	1.425357	5.005541	-0.099899
C	0	1.608112	2.480971	0.387587
N	0	1.915180	-0.070521	0.555582
H	0	-1.550881	6.507280	2.456872
H	0	-2.544149	4.498807	3.217666
C	0	-1.224755	1.392301	0.208030
C	0	-0.856865	1.090397	-1.198927
N	0	-1.453054	-0.003564	-1.787011
C	0	-2.148003	0.548117	0.836242
N	0	-2.884357	-0.188573	1.383574
H	0	-1.263453	-0.030101	-2.782894
O	0	1.262296	-2.703820	-0.434153
C	0	-0.067945	-3.243641	-0.608365
H	0	-0.668325	-2.569636	-1.226429
H	0	0.054647	-4.204176	-1.113407
H	0	-0.551834	-3.388963	0.362305
H	0	-2.065711	-1.912253	2.108633
O	0	-1.702257	-2.764452	2.419613
C	0	-2.322799	-3.095670	3.655729
H	0	-2.129617	-2.339494	4.429440
H	0	-3.409837	-3.224719	3.549071
H	0	-1.894185	-4.045961	3.984807
H	0	-2.409392	-0.339157	-1.562964
O	0	-4.123584	-1.038929	-1.846445
C	0	-4.114633	-1.287242	-3.230118
H	0	-3.859815	-0.382074	-3.811447
H	0	-3.376805	-2.063112	-3.506254
H	0	-5.096100	-1.635320	-3.598396
H	0	-5.209209	0.162453	-1.540391
O	0	-5.844828	0.700815	-0.961487
C	0	-5.872575	2.065317	-1.351896
H	0	-4.869978	2.516409	-1.335804
H	0	-6.297339	2.185769	-2.357580
H	0	-6.508329	2.603822	-0.642628
H	0	4.369442	-2.913438	1.048316
O	0	5.054063	-2.248554	0.773524
C	0	6.353100	-2.728567	1.112348
H	0	6.454198	-2.870780	2.195647
H	0	6.575320	-3.674176	0.601873
H	0	7.077293	-1.974590	0.791876
H	0	2.331341	-2.092178	-1.844683
O	0	3.032926	-1.569111	-2.291514
C	0	2.444505	-0.788903	-3.342710
H	0	1.988800	-1.437705	-4.100518
H	0	1.697509	-0.086018	-2.954809
H	0	3.255039	-0.224068	-3.810139
H	0	-4.604474	-2.442137	-1.103751
O	0	-5.015978	-2.995487	-0.361962
C	0	-4.354009	-4.244659	-0.218558
H	0	-4.437095	-4.847633	-1.133047
H	0	-3.292280	-4.118830	0.035090
H	0	-4.841865	-4.787782	0.596227

H	0	-2.405274	2.406329	2.285198
H	0	0.144079	6.696609	0.805832
C	0	2.869623	3.061920	0.123135
N	0	3.948620	3.458340	-0.100987
C	0	1.694989	1.078577	0.475739
H	0	1.212887	-1.820891	-0.008099
H	0	2.343076	-3.603608	0.703573
O	0	3.007303	-3.928376	1.356330
C	0	2.433390	-3.861009	2.666935
H	0	2.148692	-2.834756	2.929711
H	0	1.552340	-4.508596	2.740823
H	0	3.193239	-4.214788	3.367980
H	0	5.109304	2.044309	-0.772196
O	0	5.460320	1.166656	-1.033366
C	0	6.645583	1.348119	-1.813342
H	0	6.438139	1.930860	-2.718506
H	0	7.428785	1.845886	-1.229718
H	0	6.995956	0.354485	-2.104124
Na	0	4.169972	-0.645059	-0.526678
Na	0	-4.912374	-0.863867	0.383139

Transition State, TS(**9** → **10**) shown in Figure S2-15
E=-2159.53619074 a.u. and thermal correction=0.535828 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=144.1174i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.153785 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	2.448439	2.856615	-0.144100
O	0	-0.072329	3.010048	-2.469921
C	0	3.597398	3.721673	-0.136071
C	0	1.078919	3.279054	0.111301
C	0	3.706137	5.027885	0.249778
C	0	0.647168	4.483844	0.600555
C	0	2.714699	5.911236	0.775873
C	0	1.381092	5.660319	0.943232
H	0	4.520834	3.250193	-0.465046
C	0	2.571106	1.495541	-0.410779
N	0	1.044077	-0.513926	-0.306811
H	0	3.070308	6.896948	1.065710
H	0	0.780503	6.470407	1.350547
C	0	0.111926	2.190068	-0.216530
C	0	-0.391036	2.170982	-1.637770
N	0	-1.289290	1.138368	-1.886952
C	0	-0.900682	1.883884	0.721434
N	0	-1.771919	1.548776	1.430599
H	0	-1.621046	1.100206	-2.847552
O	0	-0.560486	-2.492067	0.955902
C	0	-1.967139	-2.377160	1.270741
H	0	-2.528140	-2.011272	0.403971
H	0	-2.306936	-3.382391	1.531501
H	0	-2.111477	-1.715107	2.130749
H	0	-2.034456	0.576057	3.166758
O	0	-2.124106	0.028221	3.969920
C	0	-3.247198	0.488141	4.711898
H	0	-3.123614	1.529108	5.042626
H	0	-4.181007	0.408020	4.137116
H	0	-3.328252	-0.149212	5.596317
H	0	-1.010059	0.224913	-1.525912
O	0	-3.722719	-1.208548	-1.496207
C	0	-3.582788	-2.440383	-2.137126
H	0	-2.923687	-2.376088	-3.024322
H	0	-3.143113	-3.211210	-1.473935
H	0	-4.548363	-2.848786	-2.490261
H	0	-4.170563	-0.000920	-2.493297
O	0	-4.294661	0.966650	-2.776494
C	0	-5.610630	1.166305	-3.275194
H	0	-5.774800	0.615684	-4.212083
H	0	-6.372146	0.857258	-2.545104
H	0	-5.732660	2.234726	-3.479144
H	0	2.558717	-3.012649	2.160218
O	0	3.237248	-3.048397	1.437618

C	0	4.363514	-3.812297	1.859377
H	0	4.852834	-3.353768	2.728420
H	0	4.079275	-4.842884	2.109642
H	0	5.073466	-3.831938	1.028155
H	0	0.040634	-3.605409	-0.362183
O	0	0.674590	-3.944473	-1.035525
C	0	-0.000088	-4.777293	-1.976193
H	0	-0.392495	-5.682313	-1.495498
H	0	-0.821897	-4.242624	-2.468253
H	0	0.733060	-5.072798	-2.731181
H	0	-4.873211	-0.894011	-0.374641
O	0	-5.317667	-0.260198	0.281377
C	0	-5.828654	-0.954298	1.406393
H	0	-6.612495	-1.668794	1.118143
H	0	-5.040949	-1.497442	1.949876
H	0	-6.269496	-0.216829	2.084235
H	0	-0.428615	4.568902	0.736282
H	0	4.704469	5.453044	0.170760
C	0	3.792802	0.859449	-0.726850
N	0	4.765926	0.281312	-1.018482
C	0	1.395187	0.637963	-0.307063
H	0	-0.218748	-1.652522	0.560057
H	0	0.466055	-2.740908	2.429526
O	0	1.137604	-2.841621	3.143707
C	0	1.087750	-1.686514	3.992808
H	0	1.510268	-0.805707	3.490521
H	0	0.060642	-1.462585	4.298318
H	0	1.688893	-1.913639	4.876754
H	0	4.732653	-1.563525	-1.721453
O	0	4.306783	-2.422279	-1.920299
C	0	4.707090	-2.866922	-3.218122
H	0	4.405141	-2.155361	-3.996633
H	0	5.791627	-3.020844	-3.265334
H	0	4.207592	-3.822213	-3.396514
Na	0	2.419454	-2.530719	-0.610347
Na	0	-3.466222	0.856114	-0.552607

The mono-anion **10** shown in Figure S2-16
E=-2159.55687368 a.u. and thermal correction=0.532186 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.172531 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	0.068544	3.286865	0.545866
O	0	-2.906672	0.697790	0.275416
C	0	0.061340	4.728281	0.554995
C	0	-0.858353	2.432491	1.272064
C	0	-0.739306	5.582045	1.253090
C	0	-1.845303	2.773461	2.147227
C	0	-1.794629	5.296986	2.184378
C	0	-2.266815	4.078033	2.573740
H	0	0.811295	5.187918	-0.085532
C	0	0.975421	2.522286	-0.167352
N	0	1.482831	0.088898	-0.399403
H	0	-2.268983	6.169187	2.627954
H	0	-3.080423	4.078913	3.295389
C	0	-0.563380	0.982415	0.900634
C	0	-1.734204	0.346269	0.063349
N	0	-1.368430	-0.583541	-0.813572
C	0	-0.351184	0.155675	2.077493
N	0	-0.151045	-0.507286	3.010967
H	0	-2.086964	-1.054626	-1.390524
O	0	1.984947	-2.505890	0.215830
C	0	0.962015	-3.391453	0.690674
H	0	0.088298	-3.373040	0.027578
H	0	1.381397	-4.400515	0.695161
H	0	0.658628	-3.129764	1.709308
H	0	0.654297	-2.000146	4.105338
O	0	1.055976	-2.792484	4.507962
C	0	0.171693	-3.296404	5.500805
H	0	0.010383	-2.574297	6.314017

H	0	-0.804228	-3.578256	5.080205
H	0	0.639154	-4.191215	5.920215
H	0	-0.371193	-0.750412	-0.953650
O	0	-5.491883	-2.333440	-0.862456
C	0	-5.632018	-3.582105	-0.240501
H	0	-4.660785	-3.982160	0.101459
H	0	-6.283501	-3.518741	0.647838
H	0	-6.074097	-4.336470	-0.914535
H	0	-4.369914	-2.098618	-1.744513
O	0	-3.595091	-1.570192	-2.247796
C	0	-3.648889	-1.799256	-3.648381
H	0	-3.345473	-2.824704	-3.900395
H	0	-4.661123	-1.629252	-4.041132
H	0	-2.963609	-1.102989	-4.144878
H	0	5.036336	-1.041507	0.581286
O	0	5.269950	-0.415875	-0.152831
C	0	6.606810	0.047518	0.000727
H	0	6.733388	0.609006	0.936091
H	0	7.324344	-0.783650	-0.016621
H	0	6.820082	0.714635	-0.838883
H	0	2.728210	-2.605945	-1.422160
O	0	3.201395	-2.330845	-2.243087
C	0	4.206345	-3.295310	-2.553707
H	0	4.931645	-3.400104	-1.736568
H	0	3.763337	-4.275130	-2.773600
H	0	4.729053	-2.942849	-3.447008
H	0	-6.703304	-1.249800	-1.009510
O	0	-7.021694	-0.286380	-1.016228
C	0	-8.207182	-0.129522	-1.778096
H	0	-8.075068	-0.472548	-2.814320
H	0	-9.047738	-0.677195	-1.330736
H	0	-8.458490	0.935350	-1.794067
H	0	-2.403491	1.948348	2.579126
H	0	-0.546546	6.640698	1.092321
C	0	1.992347	3.030682	-0.998408
N	0	2.842649	3.394918	-1.712958
C	0	0.810119	1.052682	0.017921
H	0	1.634089	-1.558897	0.104860
H	0	3.460735	-2.357307	1.242683
O	0	4.325333	-2.180783	1.684185
C	0	4.079989	-1.740618	3.027416
H	0	3.638905	-0.734894	3.042060
H	0	3.412790	-2.429536	3.554942
H	0	5.047065	-1.712429	3.536065
H	0	3.960214	2.271128	-2.869440
O	0	4.300251	1.406938	-3.178830
C	0	4.431791	1.421180	-4.600573
H	0	3.468465	1.607594	-5.092179
H	0	5.157503	2.177404	-4.923584
H	0	4.794980	0.434409	-4.897561
Na	0	3.540715	-0.110125	-1.604200
Na	0	-4.781870	-0.186458	-0.618091

Transition State, TS(**10** → **11**) shown in Figure S2-17
E=-2159.55219479 a.u. and thermal correction=0.528912 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=970.0299i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.171050 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	0.467523	0.710072	3.057636
O	0	2.429137	0.019549	0.468930
C	0	0.805808	0.652033	4.457245
C	0	0.937969	1.713357	2.118674
C	0	1.556828	1.516249	5.196231
C	0	1.694148	2.823372	2.337844
C	0	2.216740	2.730511	4.803307
C	0	2.269299	3.298575	3.564692
H	0	0.392862	-0.203130	4.988045
C	0	-0.362395	-0.194275	2.420297
N	0	-1.386322	-0.427823	0.182263
H	0	2.737816	3.252903	5.601940

H	0	2.828751	4.226758	3.476296
C	0	0.440475	1.336512	0.719696
C	0	1.604003	0.742517	-0.111829
N	0	1.644602	1.009277	-1.420664
C	0	-0.232074	2.446469	0.065816
N	0	-0.772675	3.322894	-0.472345
H	0	2.358076	0.533318	-2.007008
O	0	-2.157216	-0.001899	-2.145524
C	0	-1.385483	0.564755	-3.183166
H	0	-0.442657	0.015068	-3.333610
H	0	-1.946943	0.528164	-4.125350
H	0	-1.153886	1.624005	-2.984731
H	0	-2.067216	4.429481	-1.647460
O	0	-2.655461	4.912105	-2.255000
C	0	-2.073343	6.176056	-2.542887
H	0	-1.956138	6.793221	-1.640222
H	0	-1.094064	6.079380	-3.034149
H	0	-2.752749	6.690919	-3.227161
H	0	0.932909	1.572419	-1.866058
O	0	5.885088	-0.392698	-1.730822
C	0	6.857238	0.581899	-1.996411
H	0	6.408614	1.580307	-2.145994
H	0	7.573462	0.673422	-1.161993
H	0	7.442922	0.350863	-2.903194
H	0	4.655402	-0.372802	-2.474825
O	0	3.619693	-0.505852	-2.698568
C	0	3.444459	-1.252285	-3.894627
H	0	3.739924	-0.670728	-4.778591
H	0	4.033955	-2.179439	-3.874227
H	0	2.385836	-1.518490	-3.991169
H	0	-5.068186	-0.340160	-0.501454
O	0	-5.101990	-1.073027	0.171548
C	0	-6.411645	-1.185360	0.713926
H	0	-6.712226	-0.266044	1.234320
H	0	-7.152221	-1.412122	-0.064874
H	0	-6.399132	-2.006215	1.436561
H	0	-2.536399	-1.662896	-2.266318
O	0	-2.819679	-2.596272	-2.053873
C	0	-3.791671	-3.020901	-3.004820
H	0	-4.647580	-2.334000	-3.043829
H	0	-3.355982	-3.107537	-4.009187
H	0	-4.146452	-4.008944	-2.696746
H	0	6.211830	-1.822494	-0.995539
O	0	5.925765	-2.566717	-0.370569
C	0	6.551681	-3.797362	-0.695885
H	0	6.346377	-4.098153	-1.733236
H	0	7.639454	-3.744411	-0.553105
H	0	6.152031	-4.564441	-0.025926
H	0	1.904045	3.441217	1.466825
H	0	1.668920	1.257024	6.246792
C	0	-0.983923	-1.301471	3.032810
N	0	-1.509638	-2.236188	3.495597
C	0	-0.600731	0.108920	0.988974
H	0	-1.644677	-0.088399	-1.059414
H	0	-3.753351	0.593070	-1.928846
O	0	-4.700906	0.818585	-1.714590
C	0	-4.780490	2.197568	-1.340910
H	0	-4.248002	2.390590	-0.399548
H	0	-4.368710	2.847875	-2.119914
H	0	-5.838556	2.436889	-1.203437
H	0	-2.638178	-3.534949	2.528196
O	0	-3.122794	-3.855697	1.741551
C	0	-3.016908	-5.277737	1.656068
H	0	-1.971758	-5.597651	1.559458
H	0	-3.467200	-5.761013	2.531479
H	0	-3.564946	-5.585401	0.762404
Na	0	-3.100587	-2.142924	0.194827
Na	0	4.193688	-1.093081	-0.377545

The neutral intermediate **11** shown in Figure S2-18

E=-2159.57923435 a.u. and thermal correction=0.538709 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.192414 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	0.541136	3.682423	0.085584
O	0	-2.390051	0.908232	0.833601
C	0	0.532358	5.006547	-0.469413
C	0	-0.474040	3.117215	0.950139
C	0	-0.364264	6.015538	-0.262360
C	0	-1.577747	3.702579	1.496813
C	0	-1.534247	6.046851	0.562684
C	0	-2.054923	5.041777	1.329485
H	0	1.362517	5.226106	-1.137417
C	0	1.548017	2.747601	-0.135423
N	0	2.109683	0.518311	0.675383
H	0	-2.069562	6.993109	0.571639
H	0	-2.960804	5.274123	1.884172
C	0	-0.119097	1.636801	1.192635
C	0	-1.215572	0.755482	0.457134
N	0	-0.846616	-0.045412	-0.532978
C	0	-0.144412	1.305708	2.619702
N	0	-0.157845	1.072367	3.756896
H	0	-1.616540	-0.574367	-1.025300
O	0	1.390531	-2.077590	1.401662
C	0	0.249174	-2.651359	1.988792
H	0	-0.670889	-2.386078	1.436325
H	0	0.305707	-3.754175	2.013282
H	0	0.111800	-2.306695	3.026736
H	0	4.492299	1.427484	-2.362488
O	0	4.672106	0.469923	-2.443401
C	0	5.834255	0.263074	-3.247951
H	0	5.689084	0.655592	-4.261575
H	0	6.719994	0.728934	-2.798799
H	0	5.992879	-0.816377	-3.307866
H	0	0.118028	-0.326568	-0.718042
O	0	-3.817421	-3.575183	-0.848927
C	0	-2.766645	-4.511809	-0.636027
H	0	-1.985646	-4.109557	0.024330
H	0	-3.199075	-5.400753	-0.167336
H	0	-2.306897	-4.812224	-1.586984
H	0	-3.443003	-2.734141	-1.281586
O	0	-2.964929	-1.284301	-1.825079
C	0	-2.438191	-1.480519	-3.121080
H	0	-1.478938	-2.025422	-3.097098
H	0	-3.123768	-2.066759	-3.756256
H	0	-2.254520	-0.522017	-3.635914
H	0	4.604451	-2.504172	1.000002
O	0	5.066046	-2.112219	0.198654
C	0	6.322891	-2.747388	0.010263
H	0	6.992080	-2.576876	0.864259
H	0	6.208592	-3.829172	-0.140688
H	0	6.786469	-2.316552	-0.882724
H	0	1.438455	-2.054267	-0.071914
O	0	1.571331	-1.820805	-1.091409
C	0	1.322799	-2.967472	-1.893016
H	0	1.987699	-3.800427	-1.621746
H	0	0.282756	-3.309465	-1.795899
H	0	1.500885	-2.705116	-2.941638
H	0	-4.598906	-2.855592	0.495046
O	0	-4.934479	-2.150441	1.114626
C	0	-5.531104	-2.729554	2.269350
H	0	-6.395101	-3.351631	2.002210
H	0	-4.810381	-3.336714	2.832386
H	0	-5.872736	-1.911988	2.909842
H	0	-2.184350	3.066431	2.133657
H	0	-0.156167	6.940938	-0.795046
C	0	2.688981	2.937304	-0.941110
N	0	3.633041	3.051626	-1.618995
C	0	1.307031	1.503245	0.590334
H	0	1.743320	-0.299961	1.213491
H	0	2.709431	-2.690060	1.935806

O	0	3.635393	-3.029324	2.232988
C	0	3.913963	-2.526741	3.533723
H	0	3.932162	-1.427424	3.553796
H	0	3.168147	-2.876114	4.259594
H	0	4.896451	-2.899683	3.840684
H	0	-4.366465	-0.374640	-2.138645
O	0	-5.156273	0.204758	-1.917645
C	0	-6.322109	-0.269922	-2.581699
H	0	-7.168196	0.328321	-2.231555
H	0	-6.239037	-0.150421	-3.670235
H	0	-6.519878	-1.326693	-2.354233
Na	0	3.590837	-0.730008	-0.800741
Na	0	-4.106996	-0.353255	0.054350

Transition State, TS(**11** → **12** + **13**) shown in Figure S2-19
E=-2159.51015901 a.u. and thermal correction=0.537881 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=184.8697i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.137229 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	-1.055760	-0.549508	2.396481
O	0	-0.199990	0.625839	-0.651332
C	0	-2.287215	-0.514514	3.122088
C	0	-0.558255	-1.651993	1.604730
C	0	-3.192308	-1.523080	3.320625
C	0	-1.050939	-2.922158	1.495888
C	0	-3.158502	-2.878164	2.878697
C	0	-2.218783	-3.485489	2.088549
H	0	-2.515563	0.439763	3.592352
C	0	-0.147191	0.511112	2.330981
H	0	2.877000	0.421975	0.961423
H	0	-3.992275	-3.495226	3.202878
H	0	-2.389596	-4.532021	1.851075
C	0	0.662670	-1.147735	0.826004
C	0	0.138408	-0.598751	-0.649989
N	0	-0.583092	-1.481136	-1.388346
C	0	1.682233	-2.175537	0.701282
N	0	2.414143	-3.073763	0.629542
H	0	-1.465174	-1.121963	-1.805343
O	0	1.883951	-0.550933	-1.475448
C	0	2.075337	-1.483885	-2.524001
H	0	2.485430	-2.434373	-2.152006
H	0	1.130849	-1.687719	-3.047354
H	0	2.785407	-1.076093	-3.259384
H	0	3.927469	-4.189858	-0.238529
O	0	4.676195	-4.588048	-0.716397
C	0	5.869001	-3.954079	-0.268820
H	0	5.814581	-2.861669	-0.368795
H	0	6.097212	-4.200355	0.778694
H	0	6.683043	-4.327905	-0.896302
H	0	-0.513406	-2.475687	-1.232845
O	0	-3.013297	-0.305018	-2.298872
C	0	-3.099812	-0.497310	-3.692251
H	0	-3.681739	0.302810	-4.185268
H	0	-2.102082	-0.509053	-4.167280
H	0	-3.587669	-1.452988	-3.950863
H	0	-4.129409	0.748524	-1.739694
O	0	-4.402725	1.611433	-1.279286
C	0	-5.727219	1.540817	-0.773808
H	0	-6.463057	1.467557	-1.586189
H	0	-5.857916	0.683353	-0.099091
H	0	-5.922903	2.459884	-0.213001
H	0	3.484514	-0.418001	-0.767033
O	0	4.256189	-0.250089	-0.167883
C	0	5.206948	0.593181	-0.804160
H	0	5.646080	0.111945	-1.689524
H	0	4.767590	1.555780	-1.104984
H	0	6.005380	0.785176	-0.082668
H	0	1.990839	0.995998	-2.069267
O	0	2.085433	1.992114	-2.214445

C	0	2.718332	2.271016	-3.456456
H	0	3.722283	1.829505	-3.504732
H	0	2.123665	1.898267	-4.300754
H	0	2.812574	3.357158	-3.548409
H	0	-3.577999	-1.654179	-1.406491
O	0	-3.862170	-2.444130	-0.864563
C	0	-5.079770	-2.941154	-1.390003
H	0	-5.874853	-2.178826	-1.394155
H	0	-4.967014	-3.324755	-2.415641
H	0	-5.408212	-3.768635	-0.752210
H	0	-0.483535	-3.607711	0.870742
H	0	-4.059185	-1.258187	3.922235
C	0	-0.427670	1.836470	2.705892
N	0	-0.707683	2.963551	2.858837
C	0	1.049997	0.147659	1.580372
N	0	2.111674	0.859157	1.499468
H	0	2.932073	2.354974	2.509128
O	0	3.355830	3.202439	2.765409
C	0	2.980992	4.177918	1.819587
H	0	1.891451	4.360686	1.814546
H	0	3.469728	5.116158	2.097174
H	0	3.315164	3.923055	0.796552
H	0	-1.145837	3.476811	0.928163
O	0	-1.046005	3.534695	-0.047240
C	0	-1.429588	4.859471	-0.466712
H	0	-2.494199	5.032553	-0.277836
H	0	-0.835043	5.619917	0.051040
H	0	-1.238915	4.921294	-1.540339
Na	0	1.097252	2.433799	-0.284467
Na	0	-2.140412	1.523042	-1.192435

The conjugate base of azulene (**12**) + methyl carbamate (**13**) shown in Figure S2-20
E=-2159.59748934 a.u. and thermal correction=0.537595 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.222922 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	0.631289	0.686646	2.609590
O	0	-0.159586	-2.951583	-0.165513
C	0	1.206675	0.581956	3.881543
C	0	1.244434	1.246155	1.398409
C	0	2.476879	0.967485	4.300683
C	0	2.537188	1.749683	1.242698
C	0	3.516095	1.546320	3.563756
C	0	3.537821	1.879341	2.208950
H	0	0.568626	0.140082	4.645244
C	0	-0.677690	0.261688	2.263340
H	0	-1.944806	0.383193	-0.780969
H	0	4.430891	1.747597	4.116933
H	0	4.473488	2.290184	1.836364
C	0	0.266315	1.156877	0.367275
C	0	0.730468	-2.584658	-0.951151
N	0	2.033769	-2.531670	-0.709270
C	0	0.279147	1.726421	-0.907575
N	0	0.099408	2.226419	-1.957035
H	0	2.309175	-2.739883	0.245865
O	0	0.297762	-2.222142	-2.210417
C	0	1.254401	-1.895363	-3.243648
H	0	1.891269	-1.061919	-2.939378
H	0	1.873152	-2.769115	-3.466697
H	0	0.655169	-1.626952	-4.114941
H	0	-0.866537	3.950993	-1.375461
O	0	-1.613965	4.415937	-0.943481
C	0	-1.142303	5.618239	-0.324052
H	0	-0.380805	5.401055	0.433658
H	0	-0.732992	6.307458	-1.070841
H	0	-2.002453	6.087547	0.158713
H	0	2.769554	-1.936711	-1.236415
O	0	3.949852	-0.999062	-1.635748
C	0	4.876772	-1.566269	-2.520919
H	0	5.156502	-2.595895	-2.228309

H	0	4.489185	-1.624558	-3.557520
H	0	5.813770	-0.983047	-2.566394
H	0	4.351775	-1.393013	-0.035117
O	0	4.415152	-1.768472	0.893573
C	0	5.711373	-1.541165	1.407117
H	0	6.494482	-2.008956	0.789930
H	0	5.941334	-0.467490	1.495077
H	0	5.759004	-1.983657	2.408058
H	0	-1.683073	1.984441	-2.897910
O	0	-2.658583	1.949689	-2.821655
C	0	-3.191755	0.986087	-3.741562
H	0	-2.903889	1.231083	-4.769991
H	0	-2.863375	-0.028180	-3.487916
H	0	-4.279665	1.037746	-3.656948
H	0	-1.560736	-2.441800	-2.300135
O	0	-2.533156	-2.452945	-2.163271
C	0	-3.089164	-3.569390	-2.860762
H	0	-2.948312	-3.473806	-3.944834
H	0	-2.646860	-4.516140	-2.524257
H	0	-4.160980	-3.581015	-2.647113
H	0	3.964736	0.642758	-1.594210
O	0	3.965407	1.653737	-1.565993
C	0	3.887916	2.143734	-2.888815
H	0	4.750741	1.832647	-3.498831
H	0	2.968907	1.818391	-3.402237
H	0	3.881045	3.238847	-2.846605
H	0	2.826504	2.032868	0.229967
H	0	2.691832	0.783619	5.351461
C	0	-1.608099	-0.389307	3.086994
N	0	-2.427218	-0.954602	3.706382
C	0	-0.931980	0.515988	0.867422
N	0	-2.052769	0.190834	0.218523
H	0	-3.578880	0.923872	0.700832
O	0	-4.312992	1.612767	0.690381
C	0	-5.316928	1.299578	1.654675
H	0	-4.884448	1.196358	2.656513
H	0	-6.038297	2.121350	1.660747
H	0	-5.840758	0.371918	1.392008
H	0	-3.185490	-2.476587	2.736488
O	0	-3.366334	-3.098666	1.998878
C	0	-3.339222	-4.437997	2.501988
H	0	-2.361823	-4.682431	2.934993
H	0	-4.122088	-4.590515	3.254150
H	0	-3.529065	-5.103132	1.655770
Na	0	-2.251512	-2.223218	0.187211
Na	0	-3.216161	2.826634	-0.794455

Transition State, TS(**11** → **14**) shown in Figure S2-21
E=-2159.56422675 a.u. and thermal correction=0.529245 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=809.4434i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.187011 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	0.808210	3.723230	-0.064620
O	0	-2.574073	1.347610	-0.284886
C	0	1.113186	5.071474	-0.451609
C	0	-0.459028	3.254264	0.459950
C	0	0.331816	6.187699	-0.355888
C	0	-1.582803	3.959101	0.779633
C	0	-0.997053	6.334236	0.155870
C	0	-1.823488	5.363977	0.651690
H	0	2.109289	5.212249	-0.865966
C	0	1.708027	2.664531	-0.140031
N	0	1.741285	0.311728	0.501885
H	0	-1.389465	7.348159	0.143091
H	0	-2.803810	5.689606	0.991475
C	0	-0.368856	1.728682	0.619472
C	0	-1.364194	1.045658	-0.439192
N	0	-0.892602	0.256600	-1.373275
C	0	-0.791779	1.302209	1.953025
N	0	-1.131762	0.979565	3.014191

H	0	-1.703953	-0.284816	-2.166519
O	0	0.564528	-2.173616	0.870679
C	0	-0.754101	-2.590794	1.098146
H	0	-1.457001	-2.135826	0.375187
H	0	-0.865838	-3.687473	1.012627
H	0	-1.105510	-2.308584	2.106238
H	0	-2.409606	0.261516	4.469281
O	0	-3.018071	-0.158202	5.103502
C	0	-2.415427	-1.357846	5.568534
H	0	-2.205867	-2.060553	4.748671
H	0	-1.480261	-1.166742	6.114898
H	0	-3.126276	-1.827409	6.254048
H	0	0.082160	-0.031387	-1.339171
O	0	-3.787492	-3.121651	-2.504259
C	0	-2.942639	-4.205402	-2.121016
H	0	-2.368627	-3.974785	-1.214310
H	0	-3.583712	-5.069371	-1.926025
H	0	-2.246770	-4.464196	-2.929191
H	0	-3.234808	-2.308806	-2.699334
O	0	-2.635785	-0.735471	-2.858910
C	0	-2.460332	-0.371145	-4.216966
H	0	-1.645930	-0.941469	-4.688249
H	0	-3.380530	-0.567764	-4.784204
H	0	-2.222660	0.700012	-4.316159
H	0	3.709623	-2.931636	1.402789
O	0	4.437047	-2.573456	0.810168
C	0	5.603756	-3.371599	0.949066
H	0	5.994240	-3.338713	1.975105
H	0	5.411613	-4.418170	0.676406
H	0	6.367906	-2.969323	0.276521
H	0	1.084844	-2.192872	-0.576090
O	0	1.581496	-2.027179	-1.469054
C	0	1.437428	-3.151698	-2.322159
H	0	1.817989	-4.070177	-1.851637
H	0	0.386568	-3.313173	-2.602236
H	0	2.009917	-2.965684	-3.237443
H	0	-4.975413	-2.396233	-1.476292
O	0	-5.462022	-1.694452	-0.964986
C	0	-6.504777	-2.271622	-0.181795
H	0	-7.244599	-2.773119	-0.817653
H	0	-6.106374	-2.988275	0.547047
H	0	-6.997543	-1.460163	0.359660
H	0	-2.410198	3.375091	1.170351
H	0	0.788889	7.108753	-0.711291
C	0	3.030285	2.734683	-0.623454
N	0	4.122474	2.748989	-1.036871
C	0	1.128443	1.419013	0.357557
H	0	1.146105	-0.481887	0.842146
H	0	1.598026	-2.939639	1.718152
O	0	2.361566	-3.387376	2.250446
C	0	2.289569	-2.959920	3.603965
H	0	2.394483	-1.869013	3.696237
H	0	1.337238	-3.258103	4.062425
H	0	3.103645	-3.438274	4.158403
H	0	4.955309	1.054056	-1.638484
O	0	5.057543	0.087274	-1.742452
C	0	6.377009	-0.211431	-2.200169
H	0	6.569736	0.244772	-3.178676
H	0	7.135778	0.126607	-1.483604
H	0	6.442029	-1.297722	-2.299522
Na	0	3.452202	-1.060693	-0.550244
Na	0	-4.064366	0.009848	-1.286324

The E1cB intermediate **14** shown in Figure S2-22
E=-2159.57989686 a.u. and thermal correction=0.537777 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.194548 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	2.045907	3.362686	-0.135145
O	0	-2.060210	1.979358	0.111230

C	0	2.772919	4.566745	-0.418778
C	0	0.705320	3.285904	0.414048
C	0	2.390950	5.864550	-0.226077
C	0	-0.139015	4.289543	0.794085
C	0	1.171082	6.391278	0.304484
C	0	0.074134	5.702483	0.745527
H	0	3.765655	4.412094	-0.836446
C	0	2.539922	2.079224	-0.348990
N	0	1.764431	-0.209265	-0.027459
H	0	1.118921	7.476051	0.357973
H	0	-0.758225	6.300306	1.109668
C	0	0.310954	1.807052	0.501369
C	0	-0.996877	1.554931	-0.421774
N	0	-0.891372	0.975680	-1.582799
C	0	-0.082492	1.436294	1.858978
N	0	-0.446005	1.143340	2.923829
H	0	-2.382435	0.530776	-2.171340
O	0	-0.002273	-2.304530	0.475367
C	0	-1.387231	-2.420323	0.345909
H	0	-1.745321	-1.999276	-0.614084
H	0	-1.731468	-3.471910	0.380870
H	0	-1.924783	-1.887745	1.154316
H	0	-2.525436	0.725606	2.618280
O	0	-3.400829	0.343545	2.417657
C	0	-3.724042	-0.620678	3.422736
H	0	-2.967737	-1.412889	3.473483
H	0	-3.823244	-0.146501	4.406447
H	0	-4.682898	-1.062076	3.140954
H	0	0.037661	0.626993	-1.802649
O	0	-4.858497	-1.913838	-2.522315
C	0	-4.214053	-3.173001	-2.723221
H	0	-3.410045	-3.337869	-1.994748
H	0	-4.973997	-3.948178	-2.598099
H	0	-3.801648	-3.245071	-3.737047
H	0	-4.199165	-1.182081	-2.607375
O	0	-3.381587	0.359580	-2.301105
C	0	-3.922829	1.441099	-3.064203
H	0	-3.540156	1.430414	-4.092156
H	0	-5.010122	1.322336	-3.090894
H	0	-3.674760	2.403524	-2.599496
H	0	2.772385	-3.211214	1.943423
O	0	3.655306	-3.059309	1.496431
C	0	4.688300	-3.701349	2.229689
H	0	4.779191	-3.289337	3.244146
H	0	4.519682	-4.784626	2.301183
H	0	5.630012	-3.527701	1.700197
H	0	0.835833	-2.953260	-0.682768
O	0	1.541974	-3.294990	-1.345661
C	0	1.436685	-4.706153	-1.449533
H	0	1.524712	-5.195302	-0.468753
H	0	0.482638	-5.006863	-1.906109
H	0	2.248172	-5.065219	-2.092545
H	0	-5.470266	-1.355771	-0.978531
O	0	-5.600182	-0.841299	-0.141494
C	0	-6.843153	-1.188883	0.460876
H	0	-7.685815	-0.973722	-0.208688
H	0	-6.870508	-2.249666	0.742257
H	0	-6.950689	-0.583242	1.364825
H	0	-1.108913	3.967404	1.163572
H	0	3.124355	6.613983	-0.516310
C	0	3.801058	1.749762	-0.886590
N	0	4.829853	1.424702	-1.333826
C	0	1.579000	1.049953	0.043080
H	0	0.948933	-0.801817	0.260227
H	0	0.644931	-2.969984	1.719457
O	0	1.190288	-3.365477	2.499000
C	0	0.863509	-2.666173	3.691792
H	0	1.019541	-1.583159	3.590269
H	0	-0.182790	-2.841348	3.980241
H	0	1.505889	-3.040852	4.495814
H	0	5.271174	-0.493029	-1.659394

O	0	5.147450	-1.462426	-1.690844
C	0	5.678149	-1.968669	-2.917052
H	0	5.165344	-1.536000	-3.785222
H	0	6.754466	-1.772578	-2.993023
H	0	5.515981	-3.049247	-2.912846
Na	0	3.254387	-2.048071	-0.491254
Na	0	-3.743850	0.455735	0.130283

Transition State, TS(**14** → **12** + **15**) shown in Figure S2-23
E=-2159.57107205 a.u. and thermal correction=0.5535424 a.u. by B3LYP/6-31(+)G(d) $\nu^{\ddagger}$=238.9226i cm^{-1}
SCRF=(PCM, solvent=methanol)=-2160.188419 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	1.705162	3.599553	0.025259
O	0	-2.049563	1.926990	-0.428122
C	0	2.174699	4.852921	-0.457367
C	0	0.441950	3.350694	0.720099
C	0	1.588909	6.092700	-0.355376
C	0	-0.516417	4.262861	1.109593
C	0	0.367824	6.470892	0.260628
C	0	-0.544717	5.663703	0.904883
H	0	3.136136	4.816489	-0.966059
C	0	2.391415	2.388499	-0.087401
N	0	2.023803	0.064254	0.587968
H	0	0.130170	7.531180	0.218418
H	0	-1.420036	6.165397	1.312480
C	0	0.342773	1.907233	0.928538
C	0	-1.037907	1.272754	-0.596628
N	0	-0.569328	0.339525	-1.298740
C	0	-0.425758	1.401762	2.010149
N	0	-1.125505	1.015643	2.861591
H	0	-1.990153	-0.501981	-1.985635
O	0	0.389926	-2.292509	1.000303
C	0	-0.965520	-2.552411	1.199309
H	0	-1.602493	-1.990671	0.485477
H	0	-1.218018	-3.624421	1.075771
H	0	-1.297804	-2.261281	2.212798
H	0	-2.867763	0.405552	2.420035
O	0	-3.716155	0.124039	2.010187
C	0	-4.359057	-0.818195	2.871152
H	0	-3.722070	-1.693851	3.044588
H	0	-4.616555	-0.359377	3.833254
H	0	-5.277280	-1.135352	2.370391
H	0	0.343986	-0.066049	-1.092483
O	0	-4.680004	-2.763071	-1.705121
C	0	-4.286325	-4.007315	-1.118852
H	0	-3.637011	-3.856495	-0.247756
H	0	-5.199957	-4.515901	-0.802811
H	0	-3.767277	-4.636942	-1.851195
H	0	-3.885778	-2.227737	-1.928781
O	0	-2.952832	-0.674424	-2.191314
C	0	-3.232935	-0.148999	-3.498692
H	0	-2.698445	-0.715706	-4.269001
H	0	-4.308854	-0.244417	-3.663675
H	0	-2.946504	0.907190	-3.561167
H	0	3.393398	-3.474658	1.481773
O	0	4.148417	-3.215427	0.875388
C	0	5.332553	-3.900258	1.254724
H	0	5.630290	-3.657038	2.284172
H	0	5.213050	-4.989012	1.168808
H	0	6.133174	-3.581864	0.580010
H	0	0.913726	-2.395287	-0.422624
O	0	1.412379	-2.344593	-1.332652
C	0	1.144856	-3.510156	-2.091537
H	0	1.447019	-4.423855	-1.558263
H	0	0.076979	-3.593984	-2.344710
H	0	1.710567	-3.451937	-3.028487
H	0	-5.635585	-1.449888	-1.012079
O	0	-5.878908	-0.554524	-0.668986
C	0	-7.295446	-0.435003	-0.553792

H	0	-7.785983	-0.558964	-1.527195
H	0	-7.703142	-1.170220	0.151461
H	0	-7.509152	0.568273	-0.176533
H	0	-1.371689	3.849395	1.637664
H	0	2.150471	6.909152	-0.805280
C	0	3.634313	2.193932	-0.717204
N	0	4.657471	1.991363	-1.245424
C	0	1.638970	1.292497	0.527134
H	0	1.326104	-0.570999	1.016150
H	0	1.313725	-3.174306	1.851413
O	0	2.010512	-3.716330	2.390959
C	0	2.058258	-3.202370	3.714222
H	0	2.371877	-2.148165	3.734947
H	0	1.079437	-3.281947	4.206624
H	0	2.780280	-3.794030	4.287187
H	0	5.184132	0.186562	-1.747985
O	0	5.139707	-0.790187	-1.804992
C	0	6.013351	-1.256159	-2.831153
H	0	5.728675	-0.856031	-3.812601
H	0	7.055898	-0.988463	-2.618702
H	0	5.926991	-2.345412	-2.855724
Na	0	3.410613	-1.566431	-0.492830
Na	0	-3.874537	0.421619	-0.225696

The conjugate base of azulene (**12**) + cyanate ion (**15**) shown in Figure S2-24
E=-2159.63452384 a.u and thermal correction=0.531138 a.u. by B3LYP/6-31(+)G(d)
SCRF=(PCM, solvent=methanol)=-2160.258353 a.u. by B3LYP/6-311+G(d,p)

00 01

C	0	3.091026	3.597520	0.062016
O	0	-2.965388	-1.821205	-0.860846
C	0	4.129875	4.535368	0.205330
C	0	1.641592	3.853316	0.155617
C	0	4.052313	5.897442	0.467576
C	0	1.013028	5.077056	0.410126
C	0	2.925701	6.709243	0.661957
C	0	1.583544	6.332519	0.633938
H	0	5.134173	4.129762	0.095270
C	0	3.255621	2.228416	-0.204127
N	0	1.807961	0.275317	-0.523655
H	0	3.123926	7.760563	0.857643
H	0	0.868394	7.134143	0.811572
C	0	0.987568	2.616928	-0.063724
C	0	-1.786292	-2.163681	-0.903539
N	0	-0.649193	-2.492677	-0.937327
C	0	-0.396437	2.437315	-0.074404
N	0	-1.558397	2.287674	-0.083440
H	0	-4.885883	1.225310	1.007051
O	0	1.727396	-5.321284	0.782591
C	0	0.412963	-5.880308	0.772586
H	0	0.252892	-6.492073	-0.124610
H	0	0.328166	-6.524627	1.651744
H	0	-0.357261	-5.100834	0.815601
H	0	-3.235469	2.001137	-0.423645
O	0	-4.202992	1.819888	-0.586031
C	0	-4.739013	2.868131	-1.404176
H	0	-5.785307	2.624703	-1.605526
H	0	-4.684694	3.833949	-0.889099
H	0	-4.196479	2.932812	-2.353808
H	0	0.899664	-3.028862	-1.114321
O	0	-7.916725	-0.074104	0.967610
C	0	-8.879104	0.937438	1.267826
H	0	-8.599746	1.907008	0.834620
H	0	-9.828017	0.616507	0.832599
H	0	-9.009148	1.049277	2.350981
H	0	-7.039851	0.174036	1.336991
O	0	-5.240126	0.446482	1.495929
C	0	-4.483054	0.222690	2.698060
H	0	-4.851009	-0.708121	3.133760
H	0	-3.416682	0.118532	2.471529

H	0	-4.630990	1.040928	3.411426
H	0	3.772216	-2.887592	2.035775
O	0	4.201042	-2.207724	1.458397
C	0	5.531775	-1.968272	1.914714
H	0	5.538125	-1.637149	2.961424
H	0	6.154827	-2.867189	1.818843
H	0	5.953095	-1.173718	1.294145
H	0	1.796224	-4.647877	0.061957
O	0	1.844239	-3.381630	-1.193695
C	0	2.003276	-3.948488	-2.496945
H	0	3.019767	-4.345509	-2.565367
H	0	1.288906	-4.764441	-2.661969
H	0	1.856753	-3.188236	-3.274333
H	0	-7.383715	-0.587936	-0.645102
O	0	-6.794193	-0.824855	-1.401530
C	0	-7.406067	-1.841584	-2.199173
H	0	-7.621555	-2.738689	-1.606017
H	0	-8.333026	-1.477235	-2.658270
H	0	-6.700272	-2.102418	-2.991446
H	0	-0.074895	5.043057	0.437317
H	0	5.011799	6.407700	0.532524
C	0	4.472257	1.562580	-0.409093
N	0	5.461045	0.964032	-0.601425
C	0	1.964243	1.549775	-0.291089
H	0	0.820016	0.012119	-0.555295
H	0	2.449762	-4.619127	2.216072
O	0	2.876322	-4.089553	2.936571
C	0	1.858497	-3.547411	3.775445
H	0	1.143730	-2.937877	3.206094
H	0	1.314117	-4.342206	4.302016
H	0	2.350821	-2.912338	4.516420
H	0	5.481367	-0.690949	-1.628253
O	0	5.067658	-1.502991	-1.989698
C	0	5.111299	-1.448102	-3.414722
H	0	4.590438	-0.562044	-3.800879
H	0	6.145453	-1.448836	-3.781051
H	0	4.607865	-2.344359	-3.785599
Na	0	3.235085	-1.612159	-0.515575
Na	0	-4.648170	-0.499956	-0.736010