Supporting Information

Gas-phase regiocontrolled generation of charged amino acid and peptide radicals

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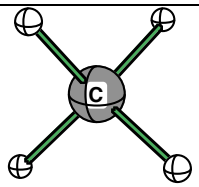
Computations

All computations were performed using the Gaussian 03 program suite (Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004).

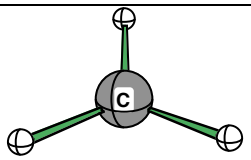
Table S1 RMP2/G3MP2Large Energies (Hartrees), B3-LYP/6-31G(*2df,p*) ZPVEs (Hartrees) and B3-LYP/6-31G(*2df,p*) Cartesian Coordinates (Å) for Species Involved in the Reactions of Table 1



CH_4 (T_d)
Energy: –40.40450
ZPVE: 0.04477

5

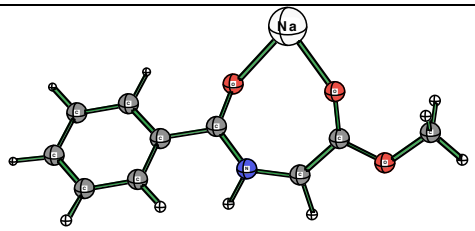
C	0.00000	0.00000	0.00000
H	-0.00000	-0.00000	1.09182
H	0.00000	-1.02938	-0.36394
H	-0.89147	0.51469	-0.36394
H	0.89147	0.51469	-0.36394



CH_3• (D_{3h})
Energy: –39.73084
ZPVE: 0.02966
S^2: 0.75395

4

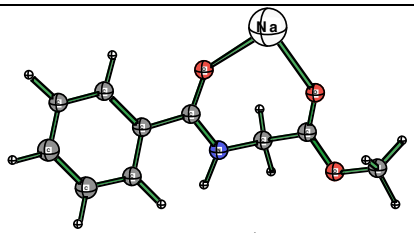
C	0.00000	0.00000	0.00000
H	0.00000	1.08126	0.00000
H	0.93640	-0.54063	0.00000
H	-0.93640	-0.54063	0.00000



R• (R = **1**+**Na**$^+$) (C_1)
Energy: –828.07054
ZPVE: 0.18810
S^2: 0.75433

25

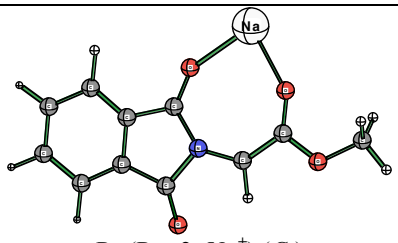
C	-0.19820040	0.89665589	-1.76830712
C	-0.17874185	0.42061009	-0.36856684
N	1.08436571	0.15037877	0.14542679
C	1.52417046	-0.34817756	1.34166484
C	0.82969043	-1.12961572	2.34227579
O	1.67837946	-1.39176031	3.33856539
C	1.18956760	-2.19781387	4.42595908
H	2.58222280	-0.20792114	1.51639613
O	-0.33132616	-1.54132070	2.33490361
H	1.83249256	0.49536763	-0.44105802
H	2.03792605	-2.31949844	5.09681774
H	0.36912924	-1.68829289	4.93680571
H	0.84764335	-3.16689033	4.05643909
O	-1.19838577	0.30467198	0.30990307
Na	-2.28751385	-0.95973905	1.66207579
C	0.81753491	0.59658881	-2.69028007
C	0.73721803	1.06882037	-3.99425294
C	-0.34975493	1.84802099	-4.38800771
C	-1.29776659	1.66452762	-2.17956857
C	-1.36662527	2.14372558	-3.48003819
H	1.64895465	-0.04613996	-2.41755840
H	1.51757002	0.82261519	-4.70497089
H	-0.40683158	2.22026886	-5.40485530
H	-2.07740444	1.89313455	-1.46319538
H	-2.21150500	2.74905393	-3.78788812



RH (R = **1**+**Na**$^+$) (C_1)
Energy: –828.72224
ZPVE: 0.20099

26

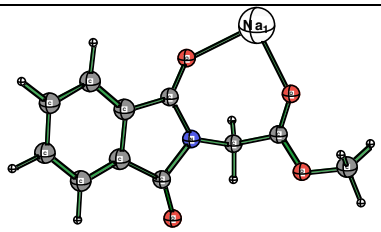
C	-0.68387860	0.66996878	-1.63798618
C	-0.69487694	0.21991017	-0.22501121
N	0.01315774	0.95305444	0.67150905
C	-0.00918535	0.69288757	2.10344168
C	0.93026749	-0.45085199	2.49721858
O	2.07529803	-0.01429455	2.96838130
C	3.06014181	-1.00296639	3.36370179
O	0.64689957	-1.63436307	2.37860822
H	0.41217764	1.82567660	0.36511469
H	3.90759106	-0.42897892	3.73205335
H	2.64997565	-1.64047648	4.14834186
H	3.34431039	-1.60807018	2.50119684
O	-1.32806175	-0.78327692	0.14335321
Na	-0.98850408	-2.59759820	1.24140670
H	0.29682203	1.60075108	2.62264923
H	-1.02254853	0.42350696	2.41451277
C	0.34833480	1.45392132	-2.17243553
C	0.30674138	1.84676213	-3.50468156
C	-0.76675408	1.46896689	-4.30983107
C	-1.74956524	0.27841843	-2.45833011
C	-1.79358932	0.68504901	-3.78561086
H	1.21002962	1.72695313	-1.57145242
H	1.11360934	2.44222362	-3.91624203
H	-0.79949383	1.78132121	-5.34775331
H	-2.54227165	-0.32825329	-2.03765935
H	-2.62766365	0.39062637	-4.41239372



R• (R = **2**+**Na**$^+$) (C_1)
Energy: –940.03634
ZPVE: 0.17548
S^2: 0.75431

25

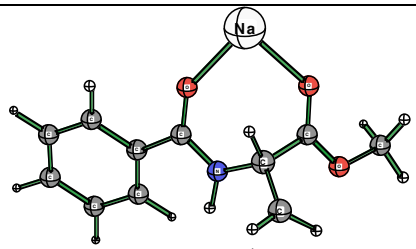
N	-0.1038027	-0.5620846	-0.0058650
C	-1.3835718	-1.0458257	-0.0104455
C	-2.6564318	-0.3613286	0.0031121
O	-2.8881441	0.8494600	0.0251541
O	-3.6271763	-1.2746189	-0.0101174
C	-4.9847390	-0.7977575	0.0033851
H	-5.1803442	-0.1852273	-0.8796494
H	-5.1722486	-0.2128633	0.9066397
H	-5.6028595	-1.6934477	-0.0078437
C	0.4583794	0.7292534	-0.0098425
C	0.9812221	-1.5702355	-0.0016193
C	1.9215229	0.5580150	-0.0043469
C	2.2336043	-0.8028840	0.0004250
C	3.5436562	-1.2507980	0.0054238
C	2.9136227	1.5259491	-0.0046639
C	4.5497914	-0.2796358	0.0055357
C	4.2397079	1.0844035	0.0005488
H	2.6698469	2.5815493	-0.0088945
H	3.7737372	-2.3094793	0.0089887
H	5.0440778	1.8112689	0.0006293
H	5.5891457	-0.5878866	0.0093950
O	0.7634111	-2.7434569	-0.0005473
O	-0.1532561	1.7856121	-0.0182162
H	-1.4138576	-2.1279236	-0.0187113
Na	-2.0581947	2.8170633	0.0122945



RH (R = **2**+**Na**$^+$) (C_1)
Energy: –940.68899
ZPVE: 0.18865

26

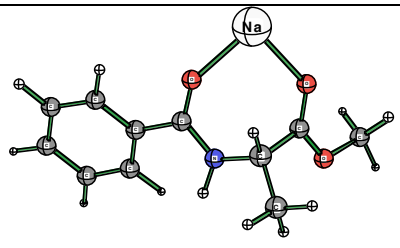
C	-1.47097	-0.61252	1.13931
Na	-1.88311	2.89737	0.36870
N	-0.14530	-0.39976	0.58778
C	-2.58668	-0.19162	0.18099
O	-2.84948	0.97525	-0.08063
O	-3.23049	-1.21790	-0.31531
C	-4.32219	-0.95405	-1.23302
H	-3.94557	-0.43406	-2.11533
H	-5.08354	-0.34943	-0.73784
H	-4.71331	-1.93404	-1.49696
H	-1.55355	-1.67935	1.35156
H	-1.58503	-0.04081	2.06579
C	0.71416	-1.50448	0.25195
C	2.00738	-0.88511	-0.12255
C	1.88990	0.50106	0.01833
C	2.95116	1.34871	-0.25109
C	4.14920	0.76191	-0.67231
C	4.26490	-0.62308	-0.81450
C	3.18749	-1.47333	-0.53926
H	3.27112	-2.54858	-0.64418
H	5.20782	-1.04632	-1.14202
H	5.00406	1.39192	-0.89060
H	2.85975	2.42218	-0.13435
C	0.51713	0.80682	0.47449
O	0.01949	1.90539	0.71078
O	0.36808	-2.65027	0.30763



R• (R = **3**+**Na**$^+$) (C_1)
Energy: –867.27364
ZPVE: 0.21350
S^2: 0.75386

28

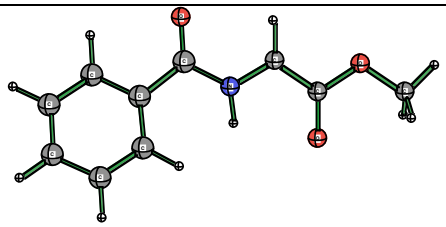
C	-0.27656	-0.46582	-1.91840
C	-0.55531	-0.36036	-0.46498
N	0.39937	-0.80395	0.39177
C	0.19815	-0.89012	1.85134
C	0.44677	0.49556	2.47275
O	1.69225	0.69102	2.83578
C	2.03366	1.98196	3.40095
O	-0.43475	1.33621	2.58335
H	1.20528	-1.28393	0.02121
H	3.09172	1.91533	3.64485
H	1.85250	2.76787	2.66588
H	1.43726	2.16341	4.29625
O	-1.62214	0.10933	-0.03261
Na	-2.31769	1.52230	1.43055
H	-0.86991	-1.09438	2.00018
C	1.02066	-1.98369	2.43916
C	1.02383	-0.54841	-2.43572
C	1.22343	-0.64849	-3.80717
C	0.12976	-0.67499	-4.67121
C	-1.36951	-0.47376	-2.79444
C	-1.16560	-0.58696	-4.16357
H	1.88933	-0.49284	-1.78319
H	2.23149	-0.70020	-4.20230
H	0.28825	-0.75823	-5.74072
H	-2.37071	-0.40756	-2.38653
H	-2.01600	-0.60579	-4.83565
H	0.76810	-3.00993	2.20290
H	1.85319	-1.77328	3.09423



RH (R = **3**+**Na**$^+$) (C_1)
Energy: –867.94671
ZPVE: 0.22860

29

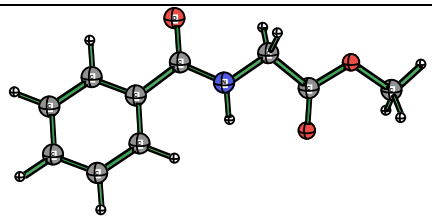
C	-0.62276	-0.26090	-1.88023
C	-0.69369	-0.12875	-0.40404
N	0.13030	-0.91160	0.33586
C	0.09452	-0.97043	1.79739
C	0.82793	0.25501	2.37202
O	2.11936	0.06595	2.51463
C	2.91008	1.17135	3.01818
O	0.26134	1.30469	2.64432
H	0.67586	-1.61541	-0.13718
H	2.54036	1.47567	3.99842
H	3.92573	0.78765	3.08718
H	2.85877	2.01145	2.32335
O	-1.48109	0.65938	0.14763
Na	-1.57709	2.11935	1.71860
H	-0.94890	-0.86528	2.10914
C	0.65881	-2.30277	2.28690
C	0.51485	-0.74381	-2.54199
C	0.52380	-0.84870	-3.92762
C	-0.60249	-0.48099	-4.66211
C	-1.74310	0.12514	-2.62675
C	-1.73451	0.00632	-4.01053
H	1.41454	-0.99960	-1.99124
H	1.41062	-1.21128	-4.43468
H	-0.59481	-0.56857	-5.74293
H	-2.61689	0.49997	-2.10787
H	-2.60959	0.29428	-4.58197
H	0.62655	-2.35318	3.37748
H	0.05800	-3.12479	1.88972
H	1.69807	-2.43156	1.97500



R• (R = **1**) (C_1)
Energy: –666.20282
ZPVE: 0.18612
S^2: 0.75532

24

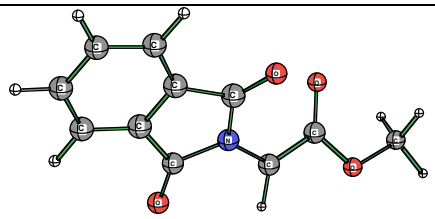
N	-0.57730066	0.23529851	-0.04416105
C	-1.83632388	0.73984511	-0.11330540
C	-2.90982688	-0.20432469	0.05531179
O	-2.73422775	-1.39831781	0.25544902
O	-4.12602361	0.37765386	-0.03290448
C	-5.23526882	-0.51067926	0.12673825
H	-5.22174814	-1.29063406	-0.63941840
H	-5.21251446	-0.98777866	1.11036028
H	-6.12705720	0.10782337	0.02457212
C	0.57924028	1.00050691	-0.14411305
O	0.51379096	2.20975711	-0.27480320
C	1.86887929	0.25415030	-0.06267993
C	3.02539827	1.01398530	0.15081382
C	4.26662120	0.39789027	0.24011042
C	4.37054358	-0.98604029	0.10641305
C	3.22761257	-1.74901069	-0.12133039
C	1.98243577	-1.13430947	-0.20464146
H	1.11381860	-1.75021166	-0.41304387
H	3.30444176	-2.82446310	-0.23897600
H	5.33998503	-1.46834563	0.17378159
H	5.15495305	0.99621801	0.41203501
H	2.91990804	2.08822683	0.24279327
H	-0.53546904	-0.75935418	0.14251315
H	-1.95939808	1.79660325	-0.28732310



RH (R = **1**) (C_1)
Energy: –666.84283
ZPVE: 0.19846

25

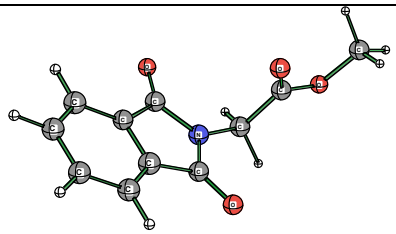
N	-0.54158816	0.22245042	-0.30038966
C	-1.84444867	0.83921529	-0.30318573
C	-2.88954584	-0.20902865	0.01950931
O	-2.64647513	-1.36692897	0.26280130
O	-4.11864323	0.31855782	-0.00363937
C	-5.18987617	-0.59059981	0.29347481
H	-5.21154821	-1.40700610	-0.43228985
H	-5.06933713	-1.00977951	1.29517176
H	-6.10281987	0.00076577	0.23265198
H	-1.89730357	1.65372044	0.42929105
H	-2.08566118	1.29288324	-1.27280147
C	0.58435808	0.98579070	-0.18511978
O	0.52920698	2.20703103	-0.17425535
C	1.88393683	0.24320177	-0.07346062
C	2.99011587	0.95917876	0.39417816
C	4.22555370	0.33767832	0.52926857
C	4.37235320	-1.00562726	0.18619735
C	3.27965138	-1.72176802	-0.29666894
C	2.04034565	-1.10135347	-0.42532577
H	1.20804119	-1.66560541	-0.83255688
H	3.39233082	-2.76318942	-0.57892841
H	5.33730128	-1.49127249	0.28815185
H	5.07606270	0.90053433	0.89936902
H	2.85145131	2.00472090	0.64239359
H	-0.53477332	-0.76232948	-0.08018182



R• (R = **2**) (C_1)
Energy: –778.15752
ZPVE: 0.17333
S^2: 0.75589

24

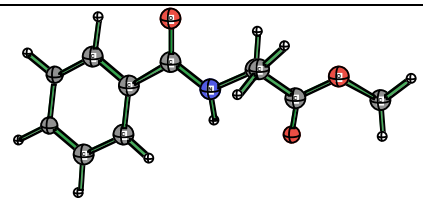
N	0.33321196	0.36061543	-0.30998327
C	0.55371201	1.69749939	-0.52627814
C	-0.22831752	2.73773759	0.12133575
O	-1.26376724	2.58428401	0.73153087
O	0.34877216	3.94522616	-0.10286455
C	-0.36790440	5.06076862	0.43263885
H	-0.47583006	4.96748315	1.51653386
H	-1.36476129	5.13155196	-0.01154448
H	0.22365435	5.94149040	0.18192938
C	-0.01947727	-0.27921787	0.92625476
C	0.58320552	-0.60545081	-1.33147075
C	-0.12029916	-1.72552368	0.59589223
C	0.25412342	-1.92032150	-0.73210941
C	0.28369972	-3.18361586	-1.29967591
C	-0.47408577	-2.78824757	1.40988138
C	-0.08162356	-4.26109938	-0.48876111
C	-0.45442592	-4.06629642	0.84479686
H	-0.75619662	-2.62506573	2.44344843
H	0.58014691	-3.32177573	-2.33289489
H	-0.73132976	-4.92309860	1.44957840
H	-0.07408827	-5.26577801	-0.89741968
O	0.97928565	-0.33661587	-2.43641857
O	-0.12818073	0.26199454	1.99045094
H	1.20539991	1.93437883	-1.35636470



RH (R = **2**) (C_s)
Energy: –778.81774
ZPVE: 0.18668

25

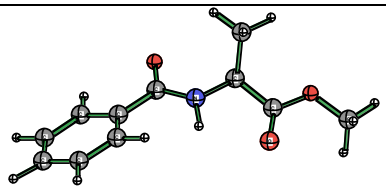
N	0.22239278	0.59479879	-0.52620925
C	1.33287459	0.54774783	-1.43641963
C	2.09514849	-0.77184126	-1.32852465
O	1.81853262	-1.67269496	-0.58253048
O	3.12100378	-0.77352490	-2.19285937
C	3.92433868	-1.96358157	-2.19326175
H	3.31770299	-2.83383758	-2.45467851
H	4.36922862	-2.12443044	-1.20842921
H	4.69881464	-1.79718718	-2.94143622
H	0.96441218	0.66188160	-2.45883689
H	2.01574498	1.37106868	-1.21290721
C	-1.04708397	0.07780334	-0.82645246
C	-1.83599857	0.21554092	0.43158408
C	-1.01131054	0.77152025	1.40897455
C	-1.47308063	1.01795726	2.68994831
C	-2.80173336	0.68561676	2.97073207
C	-3.62824448	0.12841325	1.99118051
C	-3.15295341	-0.11455418	0.69902220
H	-3.78455736	-0.54657053	-0.06862746
H	-4.65459389	-0.11963676	2.23978423
H	-3.19925899	0.86149831	3.96459566
H	-0.82272000	1.45020377	3.44164085
C	0.33365706	1.00868716	0.80995360
O	1.33083999	1.46766923	1.31157058
O	-1.37977711	-0.35975436	-1.90093841



R• (R = **3**) (C_1)
Energy: –705.39295
ZPVE: 0.21147
S^2: 0.75435

27

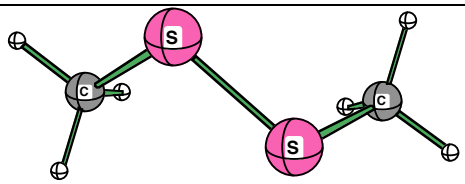
C	-0.11673370	0.05411237	-2.01045706
C	-0.89160507	-0.07251398	-0.73080742
N	-0.15919592	-0.35375222	0.39076792
C	-0.79328430	-0.37934906	1.69294243
C	0.25235780	0.08087319	2.72084844
O	-0.30594075	0.26754274	3.92092064
C	0.59330703	0.66291957	4.96896020
O	1.42477333	0.23655226	2.47902710
H	0.83810048	-0.19660504	0.40545263
H	-0.02385816	0.77220590	5.86005845
H	1.35966597	-0.10041703	5.12325425
H	1.07931938	1.60893528	4.71930693
O	-2.10445794	0.06728510	-0.69085106
H	-1.61726092	0.34710874	1.70726240
C	-1.32824839	-1.72774739	2.06307362
C	1.18329422	-0.43324686	-2.17998543
C	1.83722738	-0.28122749	-3.39927395
C	1.19937892	0.35984378	-4.45859280
C	-0.75603073	0.68071544	-3.08458463
C	-0.10040308	0.83856059	-4.29937707
H	1.68184451	-0.96290741	-1.37522313
H	2.84284125	-0.66903527	-3.52291374
H	1.71117633	0.47948576	-5.40786825
H	-1.77029239	1.03264655	-2.93835952
H	-0.60287351	1.33236125	-5.12451445
H	-2.05761127	-1.82483800	2.85635748
H	-0.91723777	-2.61135703	1.59256013



RH (R = **3**) (C_1)
Energy: –706.06614
ZPVE: 0.22670

28

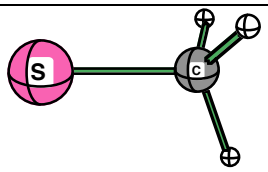
N	-0.37293936	0.26376235	-0.14384290
C	-1.76921971	0.62162430	0.00927201
C	-2.58746349	-0.40020180	-0.76784671
O	-2.11839168	-1.27188391	-1.46153056
O	-3.90040309	-0.20766179	-0.59199803
C	-4.76034942	-1.11550574	-1.29765667
H	-4.59592967	-1.03941196	-2.37508571
H	-5.77654660	-0.81669236	-1.04257230
H	-4.57131452	-2.14431771	-0.98237713
H	-2.04333074	0.54710765	1.06883053
C	-2.06462783	2.05923506	-0.45524748
H	-1.45988458	2.74578362	0.13958896
H	-3.12097913	2.29728755	-0.31322350
H	-1.80901449	2.18439933	-1.51169583
C	0.55013002	0.63990661	0.78790903
O	0.25566491	1.36405664	1.72964350
C	1.94401391	0.11683568	0.59363984
C	2.41547078	-0.40074662	-0.61721278
C	3.72353527	-0.86491536	-0.72126490
C	4.57102658	-0.81846672	0.38313170
C	4.11036603	-0.29443695	1.59016443
C	2.80697564	0.17612348	1.69213651
H	2.42807600	0.59934828	2.61477906
H	4.76965755	-0.25046660	2.45074105
H	5.58972785	-1.18302561	0.30120275
H	4.08170166	-1.25775917	-1.66696165
H	1.77866729	-0.41547895	-1.49534832
H	-0.19436271	-0.50590976	-0.77204664



MeSSMe (C_2)
Energy: –875.04652
ZPVE: 0.07713

10

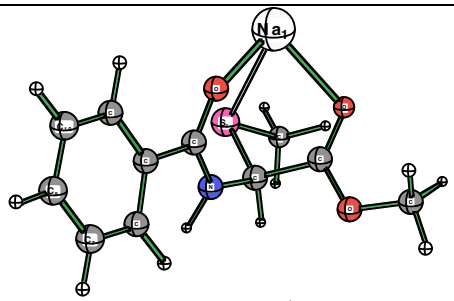
S	-0.80758	0.64115	0.49135
S	0.80758	-0.64115	0.49135
C	-1.91137	-0.05348	-0.79185
C	1.91137	0.05348	-0.79185
H	-2.81703	0.55977	-0.77179
H	2.81703	-0.55977	-0.77179
H	-1.45720	0.01096	-1.78183
H	1.45720	-0.01096	-1.78183
H	-2.16648	-1.08733	-0.55682
H	2.16648	1.08733	-0.55682



MeS• (C_s)
Energy: –437.46758
ZPVE: 0.03546
S^2: 0.75384

5

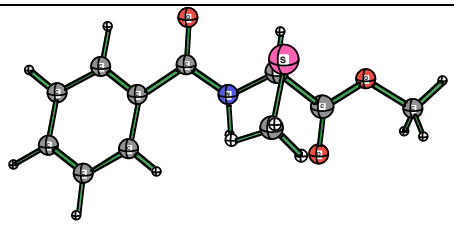
C	0.98297	0.24152	-0.45574
S	-0.61114	-0.15406	0.29071
H	1.55854	-0.65907	-0.67668
H	1.55854	0.93000	0.16543
H	0.76337	0.74488	-1.40559



MeSR (R = **1**+**Na**$^+$) (C_1)
Energy: –1265.65853
ZPVE: 0.22903

30

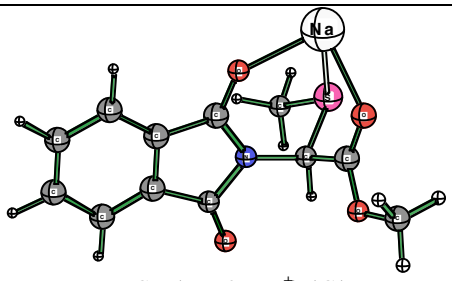
C	2.31036	-0.08486	-0.01079
C	0.84390	-0.22263	0.13894
N	0.07161	0.11450	-0.93708
C	-1.37161	0.03173	-0.95295
C	-1.99837	0.97939	0.10142
O	-1.92758	2.22485	-0.31633
C	-2.44998	3.25277	0.56454
O	-2.49862	0.63104	1.15349
H	0.52885	0.25441	-1.82404
H	-2.32083	4.18621	0.02097
H	-3.50423	3.06264	0.77092
H	-1.88343	3.26356	1.49714
O	0.31596	-0.62592	1.18295
Na	-1.59309	-1.23696	2.04258
H	-1.69789	0.39812	-1.92803
S	-1.95990	-1.71390	-0.80324
C	2.89786	0.74988	-0.97242
C	4.28109	0.83772	-1.06702
C	5.08719	0.09190	-0.20816
C	3.12757	-0.81628	0.86089
C	4.50946	-0.73271	0.75634
H	2.28716	1.36891	-1.62175
H	4.73044	1.49274	-1.80452
H	6.16668	0.15928	-0.28661
H	2.66523	-1.45198	1.60597
H	5.13721	-1.30873	1.42659
C	-3.69313	-1.51013	-1.33521
H	-4.12756	-2.51140	-1.32796
H	-4.24951	-0.87118	-0.64761
H	-3.73507	-1.11549	-2.35239



MeSR (R = **1**) (C_1)
Energy: –1103.77368
ZPVE: 0.22716

29

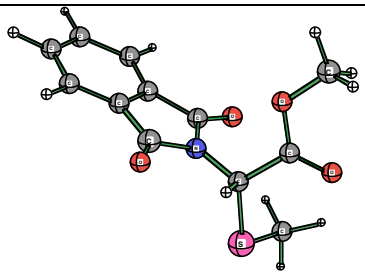
N	-0.11227500	0.01333689	-0.08614906
C	-1.21408636	-0.10862540	-0.99078905
C	-1.70841637	-1.54347291	-0.97689374
O	-0.99207373	-2.49007527	-0.73794060
O	-3.00330674	-1.62770352	-1.28501095
C	-3.53348855	-2.95824574	-1.38539395
H	-3.02524959	-3.51218541	-2.17837555
H	-4.58978718	-2.83575011	-1.62146932
H	-3.40830564	-3.49270719	-0.44091229
H	-2.00148849	0.59232340	-0.71289552
S	-0.82934727	0.34845623	-2.75380752
C	0.59048044	-0.74429403	-3.07998521
H	0.89128047	-0.54361481	-4.11002778
H	0.32330292	-1.79747691	-2.97833429
H	1.42112497	-0.50109077	-2.41453739
C	0.08016730	1.15031570	0.65969000
O	-0.66056535	2.11375305	0.55830261
C	1.24178607	1.12997911	1.60832890
C	2.28959260	0.20619074	1.53740905
C	3.33385176	0.25523781	2.45617054
C	3.34017721	1.22620961	3.45465410
C	2.30411815	2.15645196	3.52523575
C	1.26496390	2.11174763	2.60425865
H	0.45331840	2.82884235	2.63083939
H	2.30887081	2.91832522	4.29750506
H	4.15383515	1.26193134	4.17146641
H	4.14478348	-0.46198177	2.38803434
H	2.32005136	-0.53890057	0.74945703
H	0.37643448	-0.84313358	0.12429482



MeSR (R = **2**+**Na**$^+$) (C_1)
Energy: –1377.62893
ZPVE: 0.21696

30

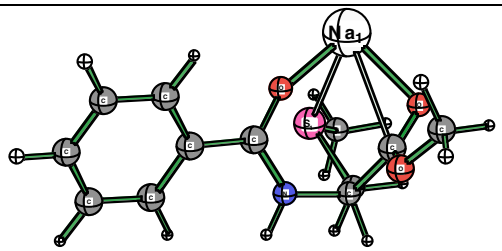
C	-1.3095866	-0.5878235	0.5702718
Na	-1.7428578	2.7010459	0.6882532
N	0.0450561	-0.3750364	0.1001027
C	-2.3508852	-0.0780667	-0.4395396
O	-2.7828782	1.0621444	-0.4506771
O	-2.6975645	-1.0195955	-1.2823379
C	-3.6640199	-0.6736145	-2.3094298
H	-3.2675104	0.1270672	-2.9356905
H	-4.5978005	-0.3566650	-1.8428467
H	-3.8044604	-1.5862527	-2.8841753
H	-1.4068685	-1.6721342	0.6562399
S	-1.7234097	0.1833185	2.1928112
C	0.9323184	-1.4949006	-0.0953209
C	2.2122307	-0.9029521	-0.5437455
C	2.0682139	0.4868510	-0.5806614
C	3.1124952	1.3129687	-0.9613893
C	4.3203392	0.6994601	-1.3093778
C	4.4633500	-0.6902048	-1.2721730
C	3.4036375	-1.5180449	-0.8850572
H	3.5069733	-2.5961884	-0.8528082
H	5.4132551	-1.1339106	-1.5483408
H	5.1614316	1.3120246	-1.6138468
H	2.9972213	2.3900645	-0.9890051
C	0.6922677	0.8299943	-0.1622283
O	0.1899191	1.9398131	-0.0521955
O	0.6106875	-2.6327294	0.1046491
C	-0.4575424	-0.5762401	3.2592396
H	-0.6621346	-0.2091626	4.2664905
H	-0.5552812	-1.6627106	3.2450801
H	0.5475513	-0.2731023	2.9633782



MeSR (R = **2**) (C_1)
Energy: –1215.74375
ZPVE: 0.21543

29

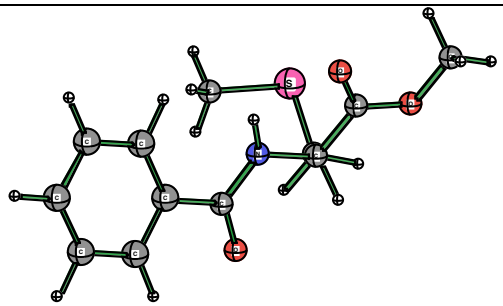
N	-0.45826	-0.10063	0.08554
C	-0.62728	-0.90655	1.27683
C	0.47466	-0.65752	2.32036
O	0.83561	-1.45329	3.14447
O	0.93030	0.60182	2.23285
C	1.94948	0.94863	3.18299
H	2.19493	1.99125	2.98341
H	2.82721	0.31316	3.04501
H	1.57834	0.82754	4.20321
H	-1.55867	-0.53600	1.72208
S	-1.00286	-2.67460	0.98411
C	0.63085	-3.46798	0.80176
H	0.40861	-4.49913	0.51754
H	1.16289	-3.45228	1.75174
H	1.21864	-2.98676	0.02214
C	-1.46346	0.77543	-0.36764
O	-2.53193	0.93573	0.16965
C	-0.90883	1.42093	-1.58942
C	0.37847	0.92845	-1.79707
C	1.15275	1.35454	-2.86196
C	0.59361	2.30093	-3.72595
C	-0.69697	2.79492	-3.51717
C	-1.47095	2.35887	-2.43754
H	-2.47238	2.73587	-2.26511
H	-1.10293	3.52881	-4.20508
H	1.16929	2.65905	-4.57270
H	2.15273	0.96489	-3.01369
C	0.68808	-0.05311	-0.71940
O	1.70007	-0.68846	-0.53794



MeSR (R = **3**+**Na**$^+$) (C_1)
Energy: –1304.88109
ZPVE: 0.25781

33

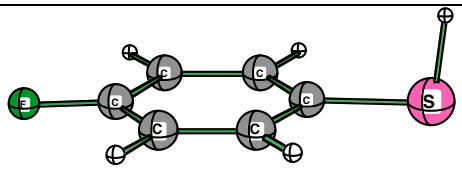
C	-0.35936	-0.63050	-2.15714
C	-0.24654	-0.31818	-0.71274
N	0.72008	-0.95932	-0.00544
C	0.95549	-0.75406	1.41950
C	-0.37165	-0.69524	2.20459
O	-0.98817	-1.85836	2.14959
C	-2.24449	-1.98068	2.85756
O	-0.76766	0.26692	2.83783
H	1.22012	-1.70875	-0.45534
H	-2.52881	-3.02617	2.75772
H	-2.11058	-1.70976	3.90574
H	-2.99485	-1.33417	2.39791
O	-1.00692	0.48311	-0.14664
Na	-1.17017	2.00184	1.43821
H	1.43935	-1.67074	1.77284
C	1.92370	0.39295	1.76801
C	0.71489	-1.13042	-2.90612
C	0.55450	-1.40342	-4.25910
C	-0.67802	-1.18566	-4.87270
C	-1.58875	-0.39578	-2.78539
C	-1.74806	-0.68071	-4.13520
H	1.69230	-1.26646	-2.45464
H	1.39205	-1.77807	-4.83626
H	-0.80194	-1.40264	-5.92794
H	-2.41129	-0.00222	-2.20070
H	-2.70516	-0.50755	-4.61398
H	1.91144	0.53549	2.85187
H	2.93173	0.09210	1.47046
S	1.58719	2.00658	0.95726
C	2.81276	3.02992	1.83437
H	2.72129	4.03824	1.42712
H	2.61564	3.04951	2.90777
H	3.82028	2.65819	1.63884



MeSR (R = **3**) (C_1)
Energy: –1142.99659
ZPVE: 0.25587

32

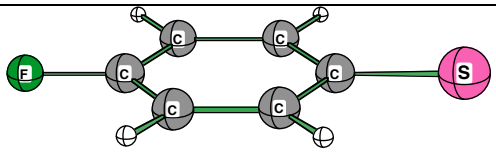
N	0.24294637	-0.01765907	0.23299445
C	1.34190716	-0.79488005	-0.30176888
C	2.40080512	0.19005183	-0.78532339
O	2.32454278	1.38838784	-0.65854981
O	3.43329808	-0.44616395	-1.34696845
C	4.48149423	0.39715296	-1.85135227
H	4.08985396	1.07059037	-2.61672757
H	5.22294191	-0.27850895	-2.27619755
H	4.91745936	0.98874639	-1.04301193
H	1.78393927	-1.39325762	0.50890161
C	0.92626720	-1.79751195	-1.39701412
H	0.13904156	-2.43990507	-0.99834532
H	1.78669835	-2.42390637	-1.64000085
S	0.38700638	-1.07138589	-2.98482132
C	-1.38329963	-0.75970285	-2.67983661
H	-1.80272220	-0.42716213	-3.63187949
H	-1.53311727	0.01484964	-1.92796534
H	-1.88685133	-1.67957045	-2.37366352
C	-0.59644068	-0.56371097	1.16352369
O	-0.54132322	-1.75170204	1.45322956
C	-1.59183487	0.36264008	1.79829744
C	-1.88527336	1.64153658	1.31283165
C	-2.82272546	2.44079644	1.96048218
C	-3.47373113	1.97155510	3.09894433
C	-3.19211872	0.69503669	3.58339912
C	-2.26086701	-0.10550778	2.93369150
H	-2.02988676	-1.10443952	3.28378507
H	-3.70073414	0.32398605	4.46695859
H	-4.20222947	2.59724180	3.60402359
H	-3.04673163	3.42894302	1.57298456
H	-1.40718347	2.01699938	0.41432800
H	0.37955707	0.98227000	0.18605182



FC_6H_4SH (C_s)
Energy: –728.55309
ZPVE: 0.09075

13

C	-0.00954	-1.15484	1.21316
C	-0.00954	-1.15484	-1.21316
C	-0.00939	0.23664	1.20720
C	-0.00939	0.23664	-1.20720
C	-0.00045	0.94032	0.00000
C	-0.00790	-1.82956	0.00000
H	-0.01381	-1.71829	2.13868
H	-0.01381	-1.71829	-2.13868
H	-0.01646	0.78233	2.14343
H	-0.01646	0.78233	-2.14343
S	-0.05342	2.73461	0.00000
F	-0.00933	-3.16512	0.00000
H	1.27653	2.95815	0.00000



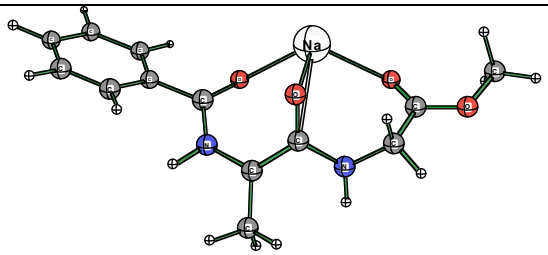
$FC_6H_4S\bullet$ (C_{2v})
Energy: –727.92490
ZPVE: 0.08235
S^2: 0.76670

12

C	1.22085	0.00000	-1.09523
C	-1.22085	0.00000	-1.09523
C	1.21700	0.00000	0.28720
C	-1.21700	0.00000	0.28720
C	0.00000	0.00000	1.01766
C	0.00000	0.00000	-1.76887
H	2.14213	0.00000	-1.66559
H	-2.14213	0.00000	-1.66559
H	2.14964	0.00000	0.83874
H	-2.14964	0.00000	0.83874
S	0.00000	0.00000	2.73385
F	0.00000	0.00000	-3.09826

Table S2 RMP2(riv)/G3MP2Large Energies (Hartrees), B3-LYP/6-31G(*d*) ZPVEs (Hartrees) and B3-LYP/6-31G(*d*) Cartesian Coordinates (Å) for Species Involved in the Energy Profile of Figure 3

Minima

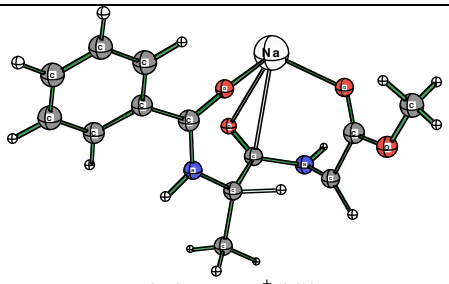


4+Na$^+$ (C_1)
Energy: –1074.95404
ZPVE: 0.27308
S^2: 0.75439

35

C	-2.4273292	-1.6593049	-1.6770573
H	-1.8504706	-2.2207826	-2.4283256
H	-1.9449305	0.8421080	-1.9979754
C	-1.5475593	-0.7850071	-0.8348153
H	-2.9889320	-2.3745248	-1.0700618
C	-0.5888353	-3.0442654	2.0242445
C	0.9168492	-3.0331400	2.3037341
O	1.2548433	-4.0293281	3.1042223
Na	1.4592685	-0.0231039	1.3245579
C	-0.1322085	1.2439117	-1.1605386
N	-1.2886971	0.4859277	-1.3115828
C	-1.0553456	-1.1729074	0.4887241
N	-0.9564518	-2.5186025	0.7273905
C	-0.1902928	2.6191194	-1.7091847
O	0.8863752	0.7730310	-0.6403766
O	-0.7623592	-0.3456535	1.3735999
O	1.7018296	-2.1923654	1.8836651
C	2.6387709	-4.1032986	3.5341470
H	-1.0727011	-3.1725747	-0.0338243
H	2.6911132	-4.9863871	4.1680744
H	3.2919459	-4.2063286	2.6656795
H	2.9021313	-3.2052248	4.0966927
H	-0.9656191	-4.0634145	2.1278355
H	-1.0595496	-2.4311248	2.8021191
H	-3.1589640	-1.0605817	-2.2340905
C	-1.3942632	3.3343396	-1.8369712
C	-1.3868509	4.6254142	-2.3598119
C	-0.1836355	5.2098876	-2.7626885
C	1.0178973	3.2217239	-2.0983430
C	1.0177601	4.5076003	-2.6292861
H	-2.3316872	2.9105721	-1.4860895
H	-2.3171842	5.1787309	-2.4431679
H	-0.1815268	6.2148740	-3.1742281
H	1.9427369	2.6641487	-1.9939880
H	1.9524724	4.9634647	-2.9412453

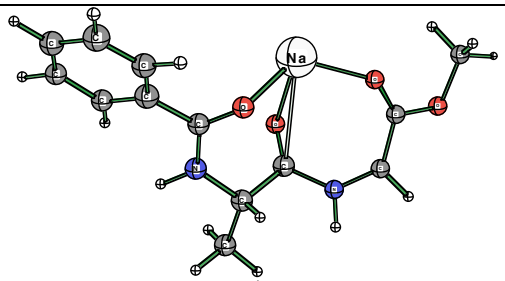
Transition Structures



TS:4↔5:Na$^+$ (C_1)
Energy: –1074.90655
ZPVE: 0.26775
S^2: 0.75678
Imaginary frequency: 1664*i* cm^{-1}

35

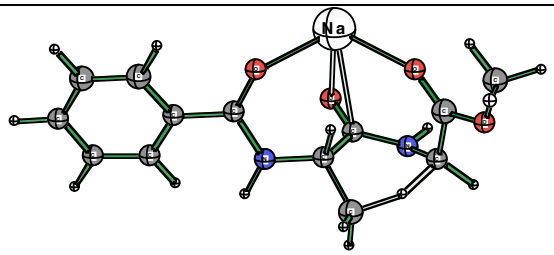
C	1.3182795	1.7315851	0.7101137
C	0.5797676	1.7134012	-0.6352487
N	-0.7363498	1.2175126	-0.6382898
C	-1.1735076	0.0968912	0.0300102
N	2.6402648	1.4561200	0.4524083
C	2.8732337	0.6153678	-0.6839913
C	3.0104452	-0.8200893	-0.3345628
O	2.7189297	-1.2765559	0.7744286
O	-0.3683831	-0.5960840	0.6701981
C	-2.6116446	-0.2379756	-0.0815208
C	-2.9916686	-1.5732138	0.1331891
C	0.7164984	3.0029771	-1.4325836
H	0.1498586	3.8113792	-0.9534909
O	0.8395989	1.9249309	1.8185905
Na	1.1366263	-0.5753587	2.2453922
O	3.4585091	-1.5480910	-1.3472052
C	3.6079409	-2.9711684	-1.1239904
H	-1.3830815	1.6471200	-1.2883821
H	3.2877892	1.4675972	1.2343939
H	3.9769893	-3.3688606	-2.0676750
H	4.3255320	-3.1495865	-0.3204637
H	2.6430232	-3.4129496	-0.8661496
H	3.5234130	0.9915564	-1.4713955
H	1.7618297	3.3131899	-1.4923861
H	0.3405317	2.8703648	-2.4530766
C	-4.3288203	-1.9437377	0.0316234
C	-5.2997574	-0.9842517	-0.2688382
C	-3.5945327	0.7242353	-0.3740484
C	-4.9325503	0.3496666	-0.4641470
H	-2.2282366	-2.3087511	0.3636203
H	-4.6160446	-2.9792984	0.1858892
H	-6.3436020	-1.2741936	-0.3436834
H	-3.3335087	1.7736935	-0.4841524
H	-5.6891319	1.0986185	-0.6763580
H	1.5230057	0.8779105	-1.1289601



5+**Na**$^+$ (C_1)
Energy: –1074.94711
ZPVE: 0.27308
S^2: 0.75439

35

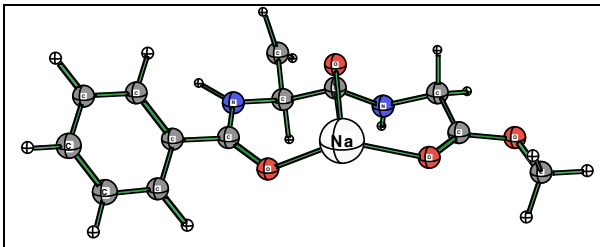
O	-0.7969073	-0.5173774	-1.0611512
C	-1.6190924	0.2226207	-0.4833380
C	-2.9899475	-0.2408251	-0.1361465
C	-3.5455705	-1.2747835	-0.9059660
H	0.1217450	2.1215525	-1.5589181
C	-0.0022451	2.0986916	-0.4668466
C	0.0332262	3.5343057	0.0864512
H	-0.0617681	3.5319286	1.1769452
O	1.0330767	0.4356251	0.9995471
C	1.1585750	1.2598939	0.1054095
N	-1.2838791	1.4950564	-0.1482174
N	2.3813591	1.5313581	-0.4945544
Na	0.7582602	-1.6568542	0.0232874
O	5.0467778	-0.7389296	0.3281623
C	3.7787743	-0.4978787	-0.0132670
O	2.9290448	-1.3833950	-0.1432753
C	5.4178653	-2.1186950	0.5383263
C	3.5955850	0.9221731	-0.2616533
H	-2.0059263	2.1027608	0.2133383
H	2.4183668	2.3605448	-1.0786548
H	6.4754920	-2.0923855	0.7949665
H	4.8325631	-2.5451948	1.3562723
H	5.2547253	-2.6956687	-0.3750021
H	4.4768310	1.5289034	-0.4288398
H	0.9672036	4.0412623	-0.1725279
H	-0.7850262	4.1222608	-0.3416285
C	-4.8286145	-1.7394784	-0.6293148
C	-5.5597408	-1.1887595	0.4265193
C	-3.7270386	0.3046845	0.9282149
C	-5.0057340	-0.1721969	1.2084080
H	-2.9690090	-1.6901999	-1.7260124
H	-5.2599181	-2.5290954	-1.2371036
H	-6.5587849	-1.5549127	0.6438408
H	-3.2957712	1.0695155	1.5692351
H	-5.5661356	0.2433232	2.0402843



TS:5↔6:**Na**$^+$ (C_1)
Energy: –1074.89498
ZPVE: 0.26794
S^2: 0.75725
Imaginary frequency: 1673*i* cm^{-1}

35

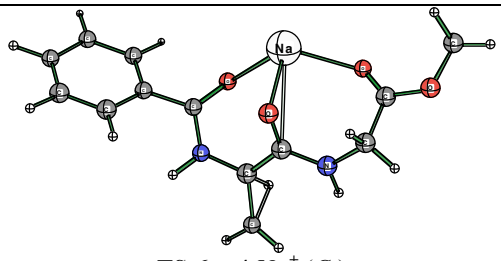
C	-3.31305927	-1.30154423	-0.07873680
H	-2.54275132	-1.60868006	-1.11235019
C	-1.22470745	-1.85037372	-1.53520190
N	-2.41030329	-1.64492228	0.97964272
C	-1.13012455	-1.16729647	0.91664990
C	-0.58394399	-0.92646853	-0.52287209
N	0.86379928	-0.89742999	-0.53364933
C	1.53125463	0.23343327	-0.16463298
O	0.89574401	1.26079354	0.14829501
C	-3.60033359	0.17328466	-0.14622573
O	-2.88669261	1.02309802	0.39277122
C	3.01570561	0.20258516	-0.18737307
C	3.69294940	1.42629341	-0.30449794
H	-1.11069936	-2.92389466	-1.38043109
O	-0.47106050	-0.88997604	1.91588595
Na	-0.81946593	1.48729755	1.52595489
O	-4.66510554	0.44365887	-0.87992906
C	-5.02147335	1.83878272	-1.05908596
H	1.37776232	-1.71901414	-0.81841801
H	-2.77920978	-1.74950371	1.92213294
H	-5.25390053	2.28880103	-0.09188276
H	-4.19853320	2.37583118	-1.53502461
H	-5.90015131	1.82527754	-1.70102136
H	-4.18271525	-1.94973242	-0.16827840
H	-1.18619182	-1.53165256	-2.57563255
C	5.08404977	1.45430631	-0.34422054
C	5.81092735	0.26482281	-0.25027134
C	3.75218883	-0.98907045	-0.08323564
C	5.14420663	-0.95503697	-0.11249087
H	3.11627443	2.34230142	-0.37468699
H	5.60228617	2.40284679	-0.44714148
H	6.89637840	0.28822257	-0.27628382
H	3.25429563	-1.94373578	0.06706915
H	5.70827675	-1.87790959	-0.01866750
H	-0.89039081	0.09413223	-0.77985599



6+Na$^+$ (C_1)
Energy: –1074.92984
ZPVE: 0.27146
S^2: 0.75415

35

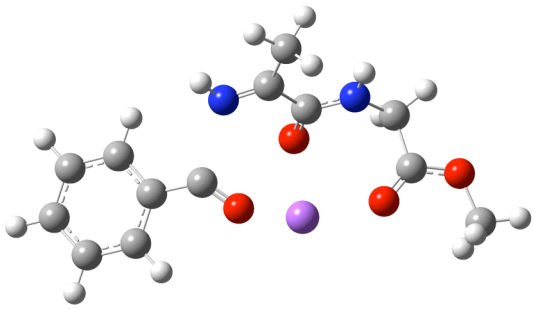
H	0.1575639	1.9490733	-1.6985470
C	-0.0513068	2.0659489	-0.6253664
C	-0.0263559	3.5124026	-0.2471138
H	0.4963763	4.2348777	-0.8616860
O	-0.7536111	-0.6399432	-0.8046956
C	-1.6372619	0.1674792	-0.4501545
C	-3.0313988	-0.2662946	-0.1628337
C	-3.4882845	-1.4455955	-0.7715436
O	0.9035557	0.7508830	1.2191736
C	1.0847271	1.3382356	0.1510527
N	-1.3505308	1.4867322	-0.3141522
N	2.3085994	1.4350233	-0.4263979
Na	0.7941849	-1.4616514	0.5191076
O	5.1121117	-0.7388181	0.0680851
C	3.8130263	-0.5043859	0.0503570
O	2.9557422	-1.3729584	-0.0461200
C	5.5443569	-2.1237516	0.0034924
C	3.5240792	0.9872535	0.2279460
H	-2.1123907	2.1371599	-0.1791846
H	2.3959615	1.8971329	-1.3218628
H	6.6313858	-2.0814519	0.0323287
H	5.1530319	-2.6747644	0.8609619
H	5.1948525	-2.5771096	-0.9257887
C	-4.7875626	-1.8913560	-0.5440255
C	-5.6350910	-1.1735115	0.3038422
C	-3.8853994	0.4476000	0.6941006
C	-5.1809954	-0.0085471	0.9269907
H	-2.8213895	-1.9907847	-1.4313702
H	-5.1407170	-2.7966140	-1.0285689
H	-6.6471210	-1.5240813	0.4836537
H	-3.5350490	1.3345794	1.2155517
H	-5.8329280	0.5399572	1.5999768
H	4.3721627	1.5670126	-0.1402387
H	3.4347606	1.1689008	1.3058253
H	-0.3866007	3.8158186	0.7306066



TS:6↔4:Na$^+$ (C_1)
Energy: –1074.87891
ZPVE: 0.26783
S^2: 0.75819
Imaginary frequency: 1809*i* cm^{-1}

35

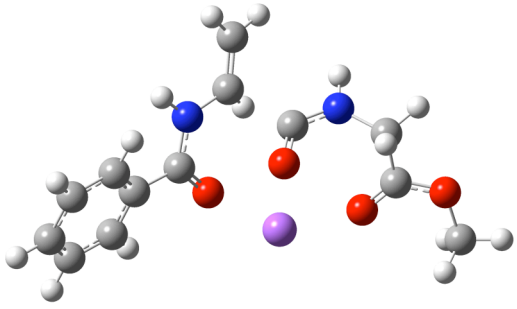
H	-2.3707732	-1.6582674	-0.0144152
C	-0.4502265	-1.6900327	-0.8066231
C	-0.7018259	-2.8466284	-1.7060404
H	0.0393619	-3.6263707	-1.8272744
C	3.3073761	-1.6930463	-0.2736190
C	3.8404197	-0.2841332	-0.5491748
O	5.1606462	-0.2834896	-0.6043833
Na	1.1921088	1.3643733	0.2662296
C	-1.7214086	0.2908055	-0.0949760
N	-1.5830882	-1.0657652	-0.2495206
C	0.8638962	-1.4556392	-0.1533236
N	1.9762498	-1.9326309	-0.7909001
C	-2.9690630	0.7683414	0.5519531
O	-0.8451932	1.0695370	-0.5079408
O	0.9582016	-0.8090013	0.9026829
O	3.1454778	0.7180357	-0.6620744
C	5.8250211	0.9953399	-0.7761875
H	1.8985630	-2.3460936	-1.7098604
H	6.8874184	0.7607124	-0.8015130
H	5.5042734	1.4570015	-1.7118359
H	5.5924002	1.6514535	0.0650827
H	3.9988855	-2.4284253	-0.6886602
H	3.2964503	-1.8233068	0.8146260
H	-1.6943147	-2.9755921	-2.1182872
H	-0.3166592	-1.5752152	-2.0531207
C	-3.7080278	-0.0185604	1.4519694
C	-4.8733941	0.4850717	2.0255666
C	-5.3125101	1.7713139	1.7030205
C	-3.4058356	2.0681733	0.2487759
C	-4.5768486	2.5620271	0.8159407
H	-3.3579878	-1.0041892	1.7479499
H	-5.4331608	-0.1219435	2.7304721
H	-6.2238406	2.1594898	2.1482309
H	-2.8267713	2.6702373	-0.4435618
H	-4.9176698	3.5623243	0.5666208



TS: loss of PhCO• from 4+Na$^+$ (C_1)
Energy: –1074.88092
ZPVE: 0.26947
S^2: 0.76469
Imaginary frequency: 287*i* cm^{-1}

35

C	0.69640000	3.37808600	1.08020500
H	1.27470500	3.02137400	1.94364300
H	-1.64704800	2.59168700	0.54219900
C	0.19884900	2.23266400	0.22747400
H	1.33184300	4.06310700	0.50479600
C	3.56586600	0.77977300	-0.82860300
C	3.82911300	-0.57454900	-0.16552100
O	5.10889800	-0.89366200	-0.23419100
Na	0.77078100	-1.56129500	-0.09982700
C	-1.89784500	-0.08777400	0.78822800
N	-1.04033300	1.93961400	0.03712100
C	1.19282200	1.31752200	-0.45463700
N	2.50929900	1.54730600	-0.19778800
C	-3.23695000	-0.34621200	0.27334500
O	-1.00770400	-0.85932600	1.05203100
O	0.83910200	0.38347500	-1.18699300
O	2.96552100	-1.29273600	0.32315000
C	5.50438400	-2.19463600	0.27492800
H	2.77863500	2.30742500	0.40995300
H	6.58166000	-2.23964500	0.12752100
H	5.25056800	-2.27044300	1.33373800
H	5.00153800	-2.98270900	-0.28923800
H	4.48694000	1.36430600	-0.83421200
H	3.28626500	0.57616600	-1.86963800
H	-0.14412500	3.95887600	1.46907100
C	-3.97236600	0.64473000	-0.39995500
C	-5.27063000	0.37319700	-0.81875800
C	-5.85131100	-0.86917600	-0.54463900
C	-3.82229700	-1.60238100	0.54101800
C	-5.12884900	-1.85358500	0.13760700
H	-3.51020100	1.59947600	-0.62058500
H	-5.83414000	1.12985900	-1.35585000
H	-6.87007200	-1.07068000	-0.86251500
H	-3.25265000	-2.35510400	1.07751600
H	-5.58493200	-2.81585700	0.35024400



TS: loss of [•CONHCH$_2$CO$_2$Me] from 6+Na$^+$ (C_1)
Energy: –1074.88774
ZPVE: 0.26957
S^2: 0.78461
Imaginary frequency: 387*i* cm^{-1}

35

H	0.24069700	1.67249300	-1.68635800
C	-0.25722400	2.21880400	-0.89170800
C	-0.07709900	3.57773700	-0.76383800
H	0.73695500	4.07227100	-1.28095100
O	-0.90138400	-0.46438000	-1.24179600
C	-1.71894100	0.27584900	-0.65877900
C	-3.02896700	-0.22649000	-0.16779900
C	-3.58780500	-1.34102000	-0.81310400
O	0.75790400	0.29989900	1.19761400
C	1.15809800	1.22923100	0.51649000
N	-1.44791500	1.59881900	-0.46986400
N	2.43376700	1.57830500	0.31292900
Na	0.77037300	-1.50666300	-0.28125600
O	5.11304000	-0.81773000	0.34599200
C	3.84664200	-0.47386100	0.20714900
O	3.00060900	-1.15771200	-0.35526800
C	5.52190700	-2.10904200	-0.17807500
C	3.56777800	0.86486900	0.89237400
H	-2.16078000	2.18033400	-0.04926400
H	2.61156000	2.38756300	-0.26682300
H	6.58659000	-2.17594200	0.03675000
H	4.97242500	-2.90555000	0.32767600
H	5.33678400	-2.14726900	-1.25303700
C	-4.81691600	-1.84593100	-0.39757900
C	-5.48978400	-1.25514400	0.67527800
C	-3.70684200	0.35872600	0.91470600
C	-4.93058400	-0.15796100	1.33460200
H	-3.05867200	-1.78645200	-1.64922300
H	-5.25238900	-2.69767600	-0.91127600
H	-6.44673600	-1.65224200	1.00077000
H	-3.26834700	1.18762500	1.46476300
H	-5.44349300	0.29032500	2.17999500
H	4.45854000	1.49339300	0.84789600
H	3.36233500	0.65380100	1.94914000
H	-0.69345400	4.18552900	-0.10833300