Supporting Information

Towards Understanding the Mechanism of Reversible Hydrogen Storage: Theoretical Study of Transition Metal Catalysed Dehydrogenation of Sodium Alanate

by Ivan Ljubić and David C. Clary

Cartesian coordinates (standard orientation, given in Å), B3LYP/6-31+G(d,p) and CCSD(T)/6-311G(2df,p) electronic energies, and B3LYP/6-31+G(d,p) harmonic vibrational wavenumbers (in cm^{-1}) of the stationary points discussed in the paper.

M1

Ti	0.000006	-0.000015	0.637932
Na	2.283851	1.589674	-0.215414
Al	1.716306	-1.476820	-0.435087
H	1.135004	-1.424141	1.171277
H	2.281919	-2.892244	-0.920520
H	1.148738	1.066556	1.492460
H	-1.148735	-1.066602	1.492420
Na	-2.283894	-1.589644	-0.215420
Al	-1.716286	1.476823	-0.435082
H	0.004021	1.311548	-0.734806
H	-0.004007	-1.311557	-0.734808
H	-2.281883	2.892277	-0.920451
H	-1.134984	1.424113	1.171277

E (B3LYP) = -1663.70027600 a.u.
E (CCSD(T)) = -1661.0342658 a.u.

77.8214	79.5521	116.8687
151.6932	172.4883	203.9621
245.0834	304.0825	340.1557
341.2152	366.5141	421.6572
457.9062	505.7208	518.7557
561.8232	568.5977	739.9245
813.4308	818.8864	896.1240
1127.0382	1156.4559	1192.4998
1218.1650	1344.3866	1367.7583
1421.2711	1439.5789	1494.4474
1506.7874	1857.6175	1861.9497

TS1

Ti	-0.102686	-0.401103	-0.788123
Na	-0.404664	1.860544	1.251192
Al	-2.423958	-0.044386	-0.003867
H	-1.474150	-0.019775	-1.903444
H	-3.984078	-0.362036	0.191367
H	-0.633691	-0.085567	-2.455035
H	0.548683	-2.019051	-0.417759
Na	1.084347	-1.622958	1.576640
Al	2.136917	0.619260	-0.457825
H	0.569946	1.393936	-0.710443
H	-1.430401	-1.442580	0.063690
H	3.385559	1.568388	-0.761917

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H        1.532224   -0.295861   -1.771901

E (B3LYP) = -1663.66965960 a.u.
E (CCSD(T)) = -1660.9982193 a.u.

  -507.7709               37.0830               68.9630
   119.9899              149.4682              171.1210
   194.5899              222.3888              247.0570
   307.9625              362.8576              391.1431
   431.2006              449.2158              470.8905
   520.0346              526.8809              654.7407
   743.3209              816.6256              868.2643
  1013.1338             1080.4051             1156.8035
  1213.9861             1330.7804             1411.2011
  1466.7714             1474.4955             1663.4304
  1705.7088             1842.8510             1867.1895
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M2

```
Ti      -0.038306   -0.332494   -0.832139
Na      -0.382379    1.858071    1.274413
Al      -2.386979    0.021515   -0.082997
H       -1.241617    0.122290   -2.171659
H       -3.934598   -0.328590    0.180491
H       -0.458871    0.093879   -2.576417
H        0.565709   -1.976990   -0.537073
Na       0.721106   -1.728829    1.564501
Al       2.210880    0.503298   -0.295867
H        0.713069    1.415219   -0.606194
H       -1.411826   -1.396892   -0.101859
H        3.545755    1.371974   -0.440112
H        1.628406   -0.230236   -1.742929

E (B3LYP) = -1663.66995516 a.u.
E (CCSD(T)) = -1660.9990535 a.u.

    47.0467               68.7213              114.3024
   143.6754              170.9142              192.6651
   219.8609              223.3441              303.0146
   325.6031              363.1138              393.7273
   420.2475              450.4588              480.6281
   502.6008              535.1156              647.4435
   807.8226              856.4545              929.3102
   989.3178             1063.9495             1158.3225
  1228.3347             1314.5171             1405.1523
  1446.4200             1463.8068             1610.4977
  1824.7443             1860.8070             2393.9218
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M3

```
Ti       0.042129   -0.342852   -0.906852
Na      -0.386252    1.937708    1.090056
Al      -2.361419    0.085939   -0.353449
H       -3.840734   -0.219587    0.218225
H        0.560661   -1.977543   -0.492750
Na       0.286476   -1.637378    1.637574
```

Al	2.249001	0.350061	-0.182405
H	0.853467	1.363689	-0.677862
H	-1.376778	-1.336459	-0.210331
H	3.668568	1.086438	-0.211516
H	1.766939	-0.345418	-1.712853

E (B3LYP) = -1662.46581088 a.u.
E (CCSD(T)) = -1659.8071407 a.u.

66.1184	70.4772	111.5906
140.3005	164.3148	189.1882
225.9867	293.9819	308.2450
369.7949	425.5239	431.4352
457.8437	479.9280	538.5339
604.3512	773.0758	867.3789
1035.4015	1117.5115	1240.2248
1297.8290	1376.9185	1407.5333
1482.6105	1798.1498	1858.6057

H_2

H	0.000000	0.000000	0.371460
H	0.000000	0.000000	-0.371460

E (B3LYP) = -1.17853934658 a.u.
E (CCSD(T)) = -1.1683401161 a.u.

4463.8747

TS2

H	-0.045563	-2.588373	0.031191
H	-1.061095	-2.283232	0.094493
Ti	-0.073900	-0.812794	-0.076939
Al	-2.417276	-0.309357	0.236743
H	-3.809308	-0.141005	1.026088
H	-1.032605	-0.158484	1.389086
H	0.976891	-0.146296	-1.463149
Na	-0.564351	1.738157	-1.575496
Na	0.898989	1.385619	1.820818
Al	2.352929	-0.535518	-0.317146
H	3.752961	-0.179295	-1.038353

E (B3LYP) = -1662.43166555 a.u.
E (CCSD(T)) = -1659.7663073 a.u.

-768.4779	54.7685	67.1557
84.9315	95.9022	124.1626
151.5573	184.2595	201.4873
260.2403	313.5098	404.4190
431.3498	448.1350	459.9656
483.2922	500.1963	549.8010
907.9563	1022.4304	1087.4088
1293.7784	1324.4936	1601.2153
1699.5698	1799.0326	1824.0408

M4

H	0.439764	-2.680739	-0.028647
H	-0.436369	-2.681264	0.028419
Ti	0.000542	-0.879023	-0.001480
Al	-2.381720	-0.363669	0.155984
H	-3.772511	0.083649	0.842876
H	-1.070329	-0.291092	1.405063
H	1.072455	-0.289520	-1.406646
Na	-0.505756	1.571813	-1.714298
Na	0.503564	1.567991	1.717249
Al	2.382106	-0.361493	-0.156083
H	3.774173	0.086742	-0.839667

E (B3LYP) = -1662.43323537 a.u.
E (CCSD(T)) = -1659.7691290 a.u.

56.6513	80.9743	85.6558
90.9680	128.5278	142.9485
180.3039	199.7391	210.0659
304.6226	375.9051	389.4372
430.4807	453.3779	468.3660
490.4757	501.6062	873.4576
912.3277	1072.6788	1080.6330
1295.7328	1329.0886	1575.0503
1798.1467	1802.8823	2440.4413

M5

Ti	0.000022	-1.017595	-0.000118
Al	2.366846	-0.382605	-0.016269
H	3.644859	0.413309	-0.609241
H	1.132658	-0.451314	-1.357112
H	-1.132536	-0.451501	1.357023
Na	0.225395	1.473113	1.717345
Na	-0.225482	1.473442	-1.717114
Al	-2.366829	-0.382687	0.016267
H	-3.644730	0.413289	0.609409

E (B3LYP) = -1661.22378393 a.u.
E (CCSD(T)) = -1658.5749422 a.u.

58.7824	87.7336	95.8738
114.0807	132.9829	181.3315
201.4780	292.0501	333.8800
353.6418	386.0331	431.4566
463.3728	491.3030	494.3336
1040.0487	1048.1807	1297.3535
1328.8293	1778.6615	1784.2245

TS3

Ti	0.033599	-0.233323	0.831190
Al	-1.875102	1.184483	-0.022743
H	-2.561150	1.034563	1.471817

H	-0.213144	1.581482	0.851660
H	0.643783	-1.495910	-0.387759
Na	-1.766618	-1.949286	-0.866301
Na	1.128775	2.055052	-0.839649
Al	2.258578	-0.829213	-0.039361
H	3.422423	-1.768963	-0.649104

E (B3LYP) = -1661.19970998 a.u.
E (CCSD(T)) = -1658.5513001 a.u.

-445.8945	35.1520	76.1164
104.3781	126.1251	155.4778
183.8006	207.8118	249.0242
322.3970	340.5394	349.4716
394.2808	505.2693	730.2986
882.0730	1125.6666	1267.8005
1349.7000	1654.4370	1795.5253

M6

Ti	0.017311	-0.059867	-1.009730
Al	2.363226	0.202524	-0.240190
H	1.312339	-1.327062	-0.882947
H	0.903872	1.504240	-0.691437
H	-1.047638	-1.387722	-0.203701
Na	0.461968	-1.647387	1.485947
Na	-0.308987	1.890671	1.231441
Al	-2.327973	-0.154571	-0.241568
H	-3.690504	-0.771883	0.363728

E (B3LYP) = -1661.23123325 a.u.
E (CCSD(T)) = -1658.5840425 a.u.

72.2725	76.9274	90.4995
133.7621	143.8516	189.3333
201.6378	212.4486	334.1008
356.7627	384.8522	458.2989
524.1842	562.5007	621.0429
741.8621	1179.9881	1254.7681
1402.6930	1442.7528	1801.3704

TS4

H	2.300556	-1.999838	-1.201282
H	-1.267268	-2.084160	0.087877
Ti	-0.007200	-0.743246	-0.021100
Al	-2.419369	-0.668358	0.592548
Na	-1.390797	1.650664	-1.360713
Na	1.260165	1.609080	1.375066
Al	2.453041	-0.516260	-0.495693
H	-0.836330	-0.140971	1.511778
H	0.960665	0.119221	-1.351188

E (B3LYP) = -1661.20613274 a.u.
E (CCSD(T)) = -1658.5472899 a.u.

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  -434.9611                31.4816                61.9066
    70.9916               103.7576               167.4870
   169.0804               186.9317               208.5830
   265.4359               368.8666               370.8546
   574.2768               729.7757               787.9210
   821.4138               983.6121              1278.2392
  1341.6650              1383.5486              1667.1856
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M7

```
H        0.658092   -1.723308    1.534421
H       -0.658092    1.723308    1.534421
Ti       0.000000    0.000000    1.208037
Al       0.000000    2.378275   -0.028036
Na      -1.760101    0.103815   -1.356672
Na       1.760101   -0.103815   -1.356672
Al       0.000000   -2.378275   -0.028036
H        1.270294    1.098818    0.465037
H       -1.270294   -1.098818    0.465037

E (B3LYP) = --1661.23696300 a.u.
E (CCSD(T)) = -1658.5891604 a.u.

   61.7973                78.1158                93.8245
  121.4606               132.0128               171.8386
  179.3299               240.5204               287.4955
  309.0664               452.6707               675.8016
  685.1077               948.0264               973.3044
 1055.3028              1064.4211              1220.9741
 1294.7423              1307.4731              1342.7522
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TS5

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H       -1.405962   -2.052994    0.366954
H       -0.433022   -2.559194    0.273611
Ti      -0.162335   -0.834675   -0.059086
Al       2.306921   -0.741016   -0.430238
Na       1.164262    1.443136    1.634737
Na      -0.454886    1.748690   -1.518044
Al      -2.484728   -0.177174    0.392109
H        0.827345   -0.223493   -1.530418
H       -0.908634    0.024935    1.401796

E (B3LYP) = -1661.19410223 a.u.
E (CCSD(T)) = -1658.5159381 a.u.

  -955.8400                49.3851                67.6375
    91.8925               112.2208               127.8146
   156.9737               173.6795               205.0868
   266.5192               372.4587               444.4819
   526.8242               545.3045               826.1870
   881.0465               910.5277              1259.9245
  1314.1796              1518.3441              1645.8297
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M8

H	-0.409465	-2.757895	0.074469
H	0.413486	-2.757332	-0.074686
Ti	0.000790	-0.898080	0.000250
Al	2.398517	-0.375564	-0.311911
Na	0.621322	1.614693	1.617810
Na	-0.624389	1.613921	-1.617717
Al	-2.397557	-0.378074	0.311379
H	0.909089	-0.221111	-1.471258
H	-0.909238	-0.223351	1.471877

E (B3LYP) = -1661.19755366 a.u.
E (CCSD(T)) = -1658.4971887 a.u.

54.7005	59.6229	91.1544
104.8716	123.1194	126.2486
163.0444	200.0255	202.5147
277.4833	364.7170	478.1292
495.5150	833.3258	850.9174
861.9361	910.4066	1269.8899
1317.8210	1445.9595	2893.2626

M9

Ti	0.000081	-1.082900	-0.000104
Al	-2.390220	-0.311266	0.247005
Na	-0.497484	1.479277	-1.637461
Na	0.497208	1.479055	1.637649
Al	2.390311	-0.311021	-0.246988
H	-0.904553	-0.314301	1.419100
H	0.904624	-0.313829	-1.419099

E (B3LYP) = -1660.00015046 a.u.
E (CCSD(T)) = -1657.3101812 a.u.

67.9095	83.1433	97.2101
127.0529	136.8580	174.1244
195.1385	257.5749	330.3707
507.2574	537.1660	888.1907
927.6869	1249.9729	1280.5372

M1Sc

Sc	0.203043	-0.994709	0.430096
Na	-1.804242	1.966510	0.131048
Al	1.157475	1.597778	0.015332
H	1.545881	0.343767	1.124842
H	2.692507	1.977488	-0.413466
H	0.206869	-1.460038	2.194703
H	1.647842	-2.092139	-0.213475
Na	3.109988	-0.550115	-0.497020
Al	-2.656730	-0.996864	-0.442278
H	-1.197953	-1.357721	-1.159288

H	1.001452	0.228395	-1.018774
H	-3.158980	0.476070	-0.951965
H	-1.874401	-0.619163	0.981393

E(B3LYP) = -1574.94754049 a.u.
E(CCSD(T) = -1572.3286545 a.u.

41.4693	49.7033	89.3157
115.5394	149.1033	176.7533
188.2165	223.7314	232.3708
256.7614	272.4689	352.1069
406.8550	417.8115	478.4404
524.6728	580.6761	622.0423
746.3634	773.3137	846.0354
878.9770	1021.5963	1031.2976
1156.8574	1258.8645	1412.7740
1495.8750	1511.5078	1590.3696
1661.6675	1694.2660	1705.9588

TS1Sc

Sc	0.134741	-0.907458	0.169497
Na	-1.767295	1.923177	-0.081195
Al	1.249350	1.533397	0.104330
H	0.975003	0.024502	1.624401
H	2.847152	1.882689	-0.095496
H	0.436456	-0.681544	2.035503
H	1.649892	-2.134546	-0.068767
Na	3.170550	-0.657132	-0.335699
Al	-2.695110	-1.007191	-0.201091
H	-1.383264	-0.512767	-1.174128
H	1.185404	0.241725	-1.075471
H	-3.502779	0.422908	-0.118544
H	-1.678353	-0.953515	1.156806

E(B3LYP) = -1574.91909914 a.u.
E(CCSD(T)) = -1572.2903594 a.u.

-667.0161	53.2377	67.9657
95.0093	124.2707	147.8728
170.1873	187.0388	219.1671
246.3848	265.1146	320.7954
390.6736	440.6074	445.4508
475.9284	628.5517	653.6019
695.9921	782.8799	837.5346
963.3239	1017.9683	1117.0100
1138.2391	1207.7900	1319.6645
1446.2441	1480.9751	1576.0906
1592.4364	1663.1196	1669.5375

M2Sc

Sc	0.116067	-0.685627	0.216171
Na	-1.961978	1.722577	-0.044037
Al	1.319456	1.708212	0.045146

H	0.762792	-0.381437	2.324999
H	2.600186	2.552081	-0.486268
H	0.198514	-0.878780	2.466573
H	1.478789	-2.088096	0.181711
Na	3.139118	-0.948887	-0.358692
Al	-2.495184	-1.175921	-0.280295
H	-1.249098	-0.232993	-1.149918
H	1.374742	0.290046	-1.033136
H	-3.615175	0.045057	-0.418541
H	-1.652242	-0.338078	1.061939

E(B3LYP) = -1574.92457946 a.u.
E(CCSD(T)) = -1572.3022325 a.u.

46.4724	60.6641	80.8903
127.1365	143.7692	151.9093
180.0669	198.8548	216.1520
235.3024	261.2178	310.3666
366.1173	429.5488	438.4566
451.6267	483.3868	523.1030
585.0987	639.7306	756.0109
846.0214	979.8243	1080.5700
1148.2090	1186.4541	1200.3739
1239.0924	1245.6131	1287.8848
1608.5948	1765.3493	3999.5194

M3Sc

Sc	-0.110261	-0.698943	-0.050264
Na	1.911241	1.729026	-0.128361
Al	-1.371430	1.658923	0.021944
H	-2.629318	2.560775	0.495871
H	-1.427105	-2.115329	-0.291936
Na	-3.178379	-0.994777	-0.051895
Al	2.547286	-1.166900	0.106848
H	1.409771	-0.212774	1.126988
H	-1.521729	0.223024	1.084921
H	3.633502	0.093950	0.070742
H	1.502760	-0.344882	-1.122508

E(B3LYP) = -1573.74198402 a.u.
E(CCSD(T)) = -1571.1299686 a.u.

47.2034	72.8775	80.3131
137.1832	148.7258	180.2270
189.3173	213.2193	259.0639
312.4420	360.1518	408.8736
424.8827	504.8760	527.3186
651.8478	780.2775	836.6693
1079.5479	1136.3528	1171.2493
1188.6209	1224.8969	1231.5455
1265.4368	1601.0479	1781.8271

TS2Sc

H	1.944039	-1.893909	0.001770
H	1.299561	-2.705705	-0.020757

Sc	0.172205	-1.153805	-0.064900
Al	-2.403252	-0.335072	0.017825
H	-3.758211	-0.014144	0.830556
H	-1.198674	-0.646729	1.319149
H	1.225878	-0.073367	-1.401810
Na	-0.560435	1.446426	-1.722121
Na	0.004013	1.332626	1.859592
Al	2.350468	0.191209	-0.035917
H	3.677934	0.864399	-0.642997

E(B3LYP) = -1573.70225513 a.u.
E(CCSD(T)) = -1571.0828981 a.u.

-860.0805	80.0398	86.0641
98.6349	133.6918	140.3575
160.9551	176.4921	182.2717
266.2322	272.6248	362.2113
409.4564	446.5380	466.0273
509.2841	601.9421	638.5932
968.7407	1087.9106	1130.7191
1143.9443	1222.6642	1405.8300
1545.8407	1806.9516	1827.7829

M4Sc

H	1.564874	2.639416	0.000452
H	0.912617	3.113377	0.047526
Sc	0.103912	1.173169	-0.033193
Al	-2.376839	0.269370	0.057919
H	-3.716577	-0.305100	-0.637746
H	-1.264055	0.516598	-1.342005
H	1.300319	0.324210	1.328199
Na	-0.292229	-1.383368	1.804500
Na	-0.075760	-1.489019	-1.739892
Al	2.340658	-0.142425	-0.061105
H	3.538906	-0.979088	0.631353

E(B3LYP) = -1573.70505809 a.u.
E(CCSD(T)) = -1571.08627350 a.u.

80.4658	87.9091	94.0113
121.5992	129.9284	136.6289
166.0288	173.6224	189.7621
276.6096	297.1119	346.4801
355.3709	459.1919	472.8469
495.6175	563.5015	707.2266
746.0617	1108.5971	1118.9345
1149.8427	1179.7009	1237.2641
1787.9574	1795.9083	3262.1377

M5Sc

Sc	0.000032	-1.246355	-0.001105
Al	2.364786	-0.185153	0.102038
H	3.606045	0.625391	-0.542336
H	1.310209	-0.539287	-1.326076

H	-1.310905	-0.544245	1.325714
Na	0.029005	1.399484	1.736030
Na	-0.029458	1.402372	-1.733908
Al	-2.364391	-0.185029	-0.102123
H	-3.606172	0.623532	0.543671

E(B3LYP) = -1572.51239245 a.u.
E(CCSD(T)) = -1569.9034356 a.u.

79.7141	95.9137	98.2659
122.6616	136.2707	170.2357
184.1438	281.8418	282.7143
332.9690	345.0683	436.7683
456.9408	475.2919	507.4609
1073.3693	1099.0305	1160.9187
1165.8883	1785.6480	1789.2991

TS3Sc

Sc	0.037960	-1.231690	-0.089221
Al	2.419535	0.038234	-0.046336
H	3.139979	-1.399558	-0.423965
H	1.159226	-0.244579	-1.371252
H	-1.172828	-0.629051	1.340919
Na	0.199163	1.254462	1.815521
Na	-0.315063	1.517909	-1.653029
Al	-2.342753	-0.246430	0.028529
H	-3.646804	0.349155	0.772011

E(B3LYP) = -1572.49739056 a.u.
E(CCSD(T)) = -1569.88533370 a.u.

-392.3040	72.6540	81.3663
91.8912	116.3021	141.4136
171.9930	183.6059	230.9175
256.2903	275.9196	356.4904
693.8948	755.9475	939.9411
1037.0509	1077.3480	1121.9714
1174.3734	1218.5928	1721.4392

M6Sc

Sc	-0.298056	-1.281563	-0.158371
Al	-2.420703	0.411796	-0.290537
H	-2.019799	-1.187350	-1.105665
H	-1.632587	-0.544776	1.120429
H	1.165688	-0.630347	-1.300506
Na	0.720819	1.652332	-1.338398
Na	-0.018916	0.966068	2.006990
Al	2.276155	-0.448053	0.121932
H	2.904046	0.944228	-0.551114

E(B3LYP) = -1572.51823155 a.u.
E(CCSD(T)) = -1569.9069621 a.u.

```
    62.4690                81.1214                94.1995
   117.3348               135.0510               179.1875
   191.6744               234.7925               254.7384
   314.2480               391.8404               485.2053
   612.4275               697.2159               928.7194
   994.6033              1089.4043              1112.2922
  1202.1561              1234.6497              1579.1794
```

TS4Sc

```
Sc       0.100405   -1.294250   -0.375898
Al       2.400153    0.210095   -0.011570
H        2.002049   -1.516200    0.136150
H        1.216236   -0.066259   -1.436586
H       -1.349440   -1.009852    0.937848
Na      -0.050790    0.622668    2.122488
Na      -0.083456    1.791867   -1.228998
Al      -2.335620    0.116787   -0.060988
H       -3.339572   -1.037779   -0.628697
```

```
E(B3LYP) = -1572.49640286 a.u.
E(CCSD(T)) = -1569.8920581 a.u.
```

```
  -431.2615                43.8564                67.3369
    73.8698                99.5073               129.7350
   154.9593               186.9347               229.1456
   241.8178               263.3938               302.6632
   664.8290               769.1360              1045.3483
  1063.1002              1100.0509              1146.6410
  1175.6580              1218.4264              1702.5074
```

M7Sc

```
H        0.621071   -1.846858    1.612961
H       -0.621071    1.846858    1.612961
Sc       0.000000    0.000000    1.234659
Al       0.000000    2.502708    0.034935
Na      -1.726886    0.113682   -1.408880
Na       1.726886   -0.113682   -1.408880
Al       0.000000   -2.502708    0.034935
H        1.324038    1.268165    0.466654
H       -1.324038   -1.268165    0.466654
```

```
E(B3LYP) = -1572.52552645 a.u.
E(CCSD(T)) = -1569.9153697 a.u.
```

```
    49.3375                68.0295                92.0122
   106.6125               119.5327               171.1149
   181.0002               222.7350               245.5090
   295.7916               411.0707               679.5277
   684.4999               938.1517               984.2632
  1049.3889              1050.7483              1088.0406
  1105.5148              1163.9929              1232.2942
```

TS5Sc

H	-2.010593	-1.793125	-0.011106
H	-1.345464	-2.678339	-0.015096
Sc	-0.210750	-1.145993	0.020501
Al	2.507428	-0.418126	-0.155485
Na	0.623560	1.391576	1.741825
Na	-0.002376	1.471047	-1.735443
Al	-2.428871	0.242075	0.115815
H	1.112407	-0.565747	-1.380228
H	-1.184861	-0.097138	1.421402

E (B3LYP) = -1572.45970114 a.u.
E (CCSD(T)) = -1569.8667690 a.u.

-1136.4691	51.8230	83.6296
91.5275	111.8237	114.4590
168.1424	171.9650	176.8935
221.3009	322.3000	510.4968
553.4105	577.1804	886.6940
1000.1780	1002.4717	1043.2735
1118.3407	1331.7353	1488.5467

M8Sc

H	0.380198	3.207775	0.451979
H	1.069299	2.907527	0.616625
Sc	0.033403	1.123112	-0.304559
Al	2.423362	0.022520	0.152211
Na	0.242438	-1.792573	-1.459697
Na	-0.364455	-1.218139	1.887284
Al	-2.473620	0.200901	-0.093195
H	1.050256	0.509582	1.274920
H	-1.205693	0.003127	-1.418458

E(B3LYP) = -1572.46464617 a.u.
E(CCSD(T)) = -1569.8589273 a.u.

54.9962	75.6670	89.4589
108.4496	119.7825	124.5259
163.4174	173.4145	181.4305
229.4098	292.3792	456.1281
509.2152	523.2714	583.7461
942.6382	984.0970	1049.3930
1056.7589	1095.4312	3903.4475

M9Sc

Sc	0.000005	-1.208566	-0.000008
Al	-2.456876	-0.247101	0.238653
Na	-0.498974	1.472460	-1.646933
Na	0.498957	1.472442	1.646947
Al	2.456883	-0.247086	-0.238652
H	-1.013520	-0.294830	1.398104
H	1.013520	-0.294789	-1.398100

E(B3LYP) = -1571.27220974 a.u.
E(CCSD(T)) = -1568.6650901 a.u.

58.4145	96.3885	103.8657
133.8342	136.1082	168.4950
179.6664	225.2455	297.5875
458.6939	477.0030	1001.2132
1058.8401	1125.2052	1137.4255