Exploring the electronic and steric effects on the dimerization of intramolecular Frustrated Lewis Pairs: A comparison between aminoboranes and aminoalanes

Supporting Information

César Barrales-Martínez[a,*], Claudio Illanes-Solis[b], Rocío Durán[a] and Julio Caballero[b]

[a]Instituto de Investigación Interdisciplinaria (I[3]), Vicerrectoría Académica, Universidad de Talca, Campus Talca, Talca, Chile.
[b]Centro de Bioinformática, Simulación y Modelado (CBSM), Facultad de Ingeniería, Universidad de Talca, Campus Talca, Talca, Chile.
[*]E-mail: cesar.barrales@utalca.cl

Table of Contents

1. Computational Details

The hybrid meta-GGA functional M06-2X[1] with the basis set 6-31G(d,p) was employed to perform geometry optimization of the stationary points of the potential energy surface (PES), which were confirmed by performing vibrational analysis, where no imaginary frequencies were found for reactants and products. The electronic energy was corrected using the triple-ζ basis set def2-TZVP, keeping the same density functional. This methodology has shown to successfully describe the reactivity of FLP in activating small molecules, such as H_2 and CO_2.[2] Gibbs free energy was computed from a statistical analysis at 298 K, employing the quasi-Rotor-Rigid-Harmonic-Oscillator (qRRHO) approximation,[3] with a threshold of 100 cm^{-1}. The implicit solvent effects were included by using the Self-Consistent Reaction Field, employing the

solvent density model (SMD).[4] Benzene was chosen as the solvent, which has a dielectric constant of 2.2706. The solvent was only included in the correction of the electronic energy at M06-2X/def2-TZVP level of theory ($E_{SMD}^{\mathrm{def2-TZVP}}$), while the geometry optimization and thermal corrections were obtained in gas phase at the M06-2X/6-31G(d,p) level of theory ($G_{thermal,gas}^{6-31G(d,p)}$). In this way, the final Gibbs free energy employed in this work is:

$$G = E_{SMD}^{\mathrm{def2-TZVP}} + G_{thermal,gas}^{6-31G(d,p)} \quad (1)$$

All electronic structure calculations were computed in Gaussian09 package.[5] The EDA calculation was performed by mixing the wavefunctions of the fragments at the dimer geometry with Multiwfn program[6], following a thermodynamic cycle and the Hess law, as described previously.[7,8] The qRRHO calculations were performed in GoodVibes package,[3,9] while the NCI index was obtained in NCIPLOT package.[10]

2. Additional computational results

Table S1. Overall energy change of dimerization (ΔE), distortion energy (ΔE_{dist}), interaction energy (ΔE_{int}), Pauli repulsion (ΔE_{Pauli}), electrostatic interaction (ΔV_{elstat}) and orbital interaction (ΔE_{oi}) for all the systems with boron and aluminum. All values are in kcal/mol.

System	ΔE	ΔE_{dist}	ΔE_{int}	ΔE_{Pauli}	ΔV_{elstat}	ΔE_{oi}
Aminoboranes						
H/H	-48.5	44.1	-92.6	234.6	-171.3	-155.9
H/CH_3	-34.9	46.3	-81.2	241.7	-173.3	-149.6
H/*t*-but	-6.9	75.1	-82.0	245.3	-177.0	-150.3
H/Ph	-33.6	52.3	-86.0	263.7	-186.2	-163.5
H/Mes	13.2	86.5	-73.3	267.3	-184.7	-155.8
CH_3/H	-27.8	65.4	-93.3	237.4	-175.4	-155.2
CH_3/CH_3	15.6	104.3	-88.7	204.0	-154.0	-138.8
CH_3/*t*-but	110.3	196.2	-88.7	260.9	-189.3	-157.4
CH_3/Ph	21.1	110.7	-89.6	223.9	-167.4	-146.1
t-but/H	37.1	127.0	-89.9	293.1	-213.3	-169.7
Ph/H	-4.3	65.1	-69.5	205.3	-143.5	-131.3
Aminoalanes						
H/H	-37.3	42.6	-79.9	115.2	-126.6	-68.5
H/CH_3	-35.7	37.9	-73.6	114.7	-124.9	-63.4
H/*t*-but	-24.7	54.3	-79.0	124.0	-134.8	-68.1
H/Ph	-38.7	42.0	-80.6	128.9	-138.3	-71.3
H/Mes	-21.0	55.0	-76.1	132.5	-136.7	-71.9
CH_3/H	-18.0	63.6	-81.6	119.1	-128.3	-72.3
CH_3/CH_3	-9.2	70.4	-79.6	112.6	-122.5	-69.7
CH_3/tbut	14.4	94.0	-79.6	118.4	-126.2	-71.8
CH_3/Ph	-12.8	76.1	-88.9	131.2	-141.9	-78.1
CH_3/Mes	10.7	94.0	-83.3	116.9	-125.2	-75.0
t-but/H	33.0	110.5	-77.4	165.3	-157.1	-85.7
Ph/H	-3.9	53.8	-57.7	93.2	-88.2	-62.7
Ph/CH_3	10.0	63.2	-53.2	87.0	-89.2	-51.0
Ph/Ph	16.1	95.0	-78.9	118.9	-117.8	-79.9

3. Cartesian coordinates of aminoboranes

3.1 Monomers

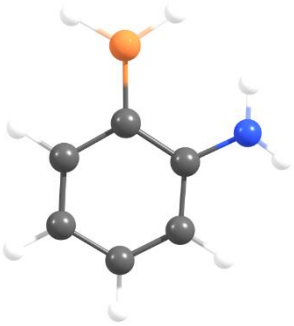

Figure S1: Computed structure of H/H (FLP)

Data for system: **H/H (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -313.0288244 A.U.
Zero-point correction= 0.129906 (Hartree/Particle)
Thermal correction to Energy= 0.137106
Thermal correction to Enthalpy= 0.138050
Thermal correction to Gibbs Free Energy= 0.099111

Optimized Geometry (XYZ coordinates in Å)

6	-1.279816	1.723933	0.563480
6	0.064843	1.891971	1.002296
5	1.138142	0.815398	0.875145
7	-1.725362	0.526783	0.063437
6	0.417260	3.141213	1.562009
1	1.442094	3.267741	1.901032
6	-0.476466	4.188096	1.681958
1	-0.174552	5.135941	2.112333
6	-2.189522	2.791969	0.683846
1	-3.214353	2.658019	0.348768
6	-1.788651	3.996303	1.231339
1	-2.510697	4.803908	1.312262
1	-2.571611	0.532661	-0.482249
1	0.938866	-0.245878	0.357041
1	2.235838	1.028385	1.292536
1	-1.033340	-0.152756	-0.208474

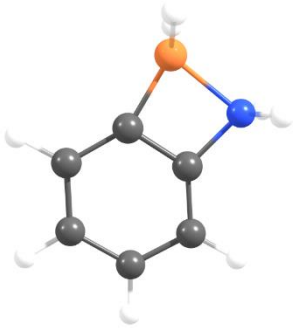

Figure S2: Computed structure of H/H (CLA)

Data for system: **H/H (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -313.0252836 A.U.
Zero-point correction= 0.131779 (Hartree/Particle)
Thermal correction to Energy= 0.138138
Thermal correction to Enthalpy= 0.139082
Thermal correction to Gibbs Free Energy= 0.101719

Optimized Geometry (XYZ coordinates in Å)

6	-1.267753	1.761523	0.616486
6	0.058362	1.877942	1.000983
5	0.385022	0.356975	0.564655
7	-1.308092	0.378568	0.131647
6	0.468867	3.100495	1.526744
1	1.491668	3.268793	1.850294
6	-0.471804	4.128521	1.634694
1	-0.169475	5.088668	2.042408
6	-2.237736	2.743760	0.701060
1	-3.265008	2.594371	0.382634
6	-1.800621	3.959640	1.231390
1	-2.499663	4.783335	1.332099
1	-1.913963	-0.241357	0.664604
1	1.017584	0.176489	-0.441344
1	0.530791	-0.464453	1.429960
1	-1.516897	0.281575	-0.859532

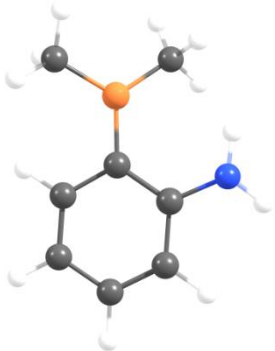

Figure S3: Computed structure of H/CH3 (FLP)

Data for system: **H/CH3 (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -391.6742132 A.U.
Zero-point correction= 0.187018 (Hartree/Particle)
Thermal correction to Energy= 0.197616
Thermal correction to Enthalpy= 0.198560
Thermal correction to Gibbs Free Energy= 0.151364

Optimized Geometry (XYZ coordinates in Å)

6	-1.554754	2.326681	-0.373498
6	-0.428234	2.218386	0.484742
5	0.692043	1.138224	0.383498
7	-1.868162	1.352659	-1.303656
6	-0.278358	3.219625	1.466167
1	0.571788	3.152487	2.139468
6	-1.140069	4.296954	1.592564
1	-0.974558	5.054153	2.350684
6	-2.440013	3.410978	-0.236641
1	-3.301882	3.473494	-0.896014
6	-2.230681	4.382553	0.725357
1	-2.927296	5.212097	0.803799
1	-2.487294	1.631885	-2.048586
1	-1.135285	0.726718	-1.590085
6	1.025463	0.328244	-0.941206
1	0.427761	-0.595910	-0.958565
1	0.827617	0.867807	-1.873167
1	2.069647	0.002005	-0.955098
6	1.630082	0.840600	1.621416
1	2.553347	1.426227	1.500867
1	1.210712	1.089577	2.598507
1	1.948212	-0.207113	1.632528

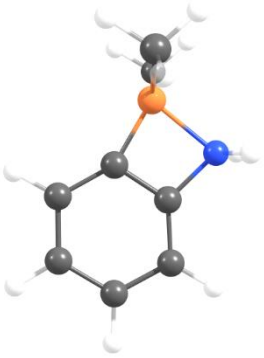

Figure S4: Computed structure of H/CH3 (CLA)

Data for system: **H/CH3 (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -391.6653272 A.U.
Zero-point correction= 0.188031 (Hartree/Particle)
Thermal correction to Energy= 0.197985
Thermal correction to Enthalpy= 0.198929
Thermal correction to Gibbs Free Energy= 0.153700

Optimized Geometry (XYZ coordinates in Å)

6	-0.382308	0.570284	-0.032634
6	-0.220492	-0.804138	0.026143
5	1.400306	-0.713297	-0.008000
7	0.998949	1.050888	-0.080036
6	-1.370423	-1.587933	0.082204
1	-1.320602	-2.671976	0.129865
6	-2.614719	-0.951418	0.076418
1	-3.521595	-1.547449	0.119699
6	-1.589010	1.247749	-0.040937
1	-1.658381	2.330499	-0.088287
6	-2.727612	0.441102	0.016096
1	-3.711227	0.899310	0.013579
1	1.246385	1.538897	-0.938622
1	1.277334	1.614369	0.720904
6	2.192888	-0.977288	1.358787
1	1.690241	-0.566222	2.242454
1	2.280771	-2.057292	1.525651
1	3.214570	-0.579928	1.330854
6	2.142252	-1.099417	-1.374150
1	2.225787	-2.190117	-1.447353
1	1.606629	-0.767945	-2.271790
1	3.163575	-0.702730	-1.419380

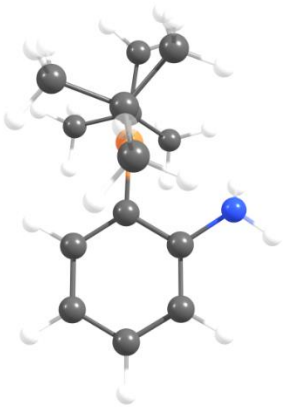

Figure S5: Computed structure of H/t-but (FLP)

Data for system: **H/t-but (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -627.5031612 A.U.

Zero-point correction= 0.358976 (Hartree/Particle)
Thermal correction to Energy= 0.377220
Thermal correction to Enthalpy= 0.378164
Thermal correction to Gibbs Free Energy= 0.314548

Optimized Geometry (XYZ coordinates in Å)

6	-0.844111	2.839728	0.627330
6	0.181060	2.474120	1.517522
5	1.506807	1.882386	0.882967
7	-0.546478	2.770500	-0.759932
6	-0.096163	2.516491	2.886476
1	0.675379	2.233236	3.599225
6	-1.358447	2.869799	3.365018
1	-1.553164	2.876735	4.432349
6	-2.106747	3.194988	1.097520
1	-2.886089	3.470120	0.390841
6	-2.366261	3.198184	2.465960
1	-3.353923	3.469128	2.825223
1	-1.356542	2.953875	-1.340661
1	0.191212	3.417365	-1.019526
6	1.489068	0.314549	0.564929
6	2.769158	2.868740	0.780131
6	4.017439	2.373717	0.038834
1	4.414696	1.445938	0.460766
1	3.818375	2.204665	-1.023274
1	4.810860	3.128807	0.108559
6	3.164482	3.149287	2.250977
1	2.362644	3.655296	2.795235
1	3.423671	2.231676	2.792170
1	4.046476	3.801359	2.270361
6	2.361009	4.214249	0.149597
1	2.193299	4.112687	-0.930037
1	1.459241	4.627780	0.613525
1	3.167278	4.947933	0.272852
6	2.316532	-0.326175	1.704646
1	3.362573	-0.004386	1.695272
1	1.896000	-0.091654	2.690515
1	2.302696	-1.417989	1.597597
6	0.074404	-0.285504	0.619183
1	0.123444	-1.370260	0.462280
1	-0.410051	-0.103878	1.582817
1	-0.559056	0.145231	-0.162163
6	2.101317	-0.069977	-0.792505
1	3.170894	0.134322	-0.850386
1	1.964056	-1.144701	-0.965517
1	1.602101	0.461706	-1.609921

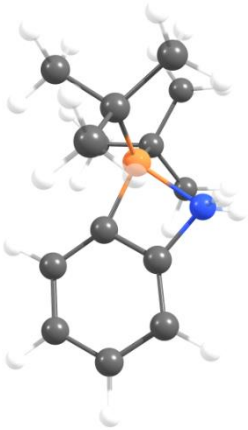

Figure S6: Computed structure of H/t-but (CLA)

Data for system: **H/t-but (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -627.502937 A.U.
Zero-point correction= 0.360281 (Hartree/Particle)
Thermal correction to Energy= 0.377515
Thermal correction to Enthalpy= 0.378459
Thermal correction to Gibbs Free Energy= 0.317911

Optimized Geometry (XYZ coordinates in Å)

6	-1.327690	2.243791	0.658377
6	-0.076712	2.679864	1.061917
5	0.656188	1.307296	0.579353
7	-1.036914	0.916215	0.113450
6	0.012250	3.945531	1.635637
1	0.961377	4.352953	1.974245
6	-1.157487	4.699387	1.777144
1	-1.107046	5.687615	2.224638
6	-2.511774	2.949032	0.773415
1	-3.467834	2.558803	0.437467
6	-2.398675	4.214317	1.355645
1	-3.284478	4.828321	1.480682
1	-1.480193	0.150324	0.617971
1	-1.233487	0.822681	-0.880918
6	1.036905	0.265156	1.784530
6	1.561050	1.494597	-0.774231
6	2.221238	0.214041	-1.302905
1	2.953692	-0.191427	-0.598508
1	1.481968	-0.570328	-1.505590
1	2.751653	0.416550	-2.243003
6	2.666975	2.520617	-0.461087
1	2.236568	3.488605	-0.182359
1	3.317452	2.195383	0.355351
1	3.300374	2.680479	-1.343542
6	0.735275	2.085282	-1.933417
1	0.049579	1.347035	-2.371487

1	0.152680	2.960300	-1.624613
1	1.396647	2.400503	-2.749892
6	0.977636	-1.213592	1.364622
1	-0.006247	-1.490397	0.962476
1	1.720662	-1.467403	0.607065
1	1.157818	-1.862801	2.231392
6	2.450189	0.566781	2.307720
1	2.671529	-0.042331	3.194105
1	3.218965	0.348479	1.560122
1	2.550792	1.619795	2.596997
6	0.077293	0.432845	2.978189
1	-0.972013	0.247263	2.710288
1	0.330260	-0.277736	3.775135
1	0.124903	1.442742	3.395641

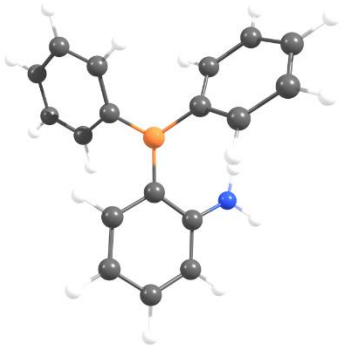

Figure S7: Computed structure of H/Ph (FLP)

Data for system: **H/Ph (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -775.1497291 A.U.
Zero-point correction= 0.296957 (Hartree/Particle)
Thermal correction to Energy= 0.313290
Thermal correction to Enthalpy= 0.314234
Thermal correction to Gibbs Free Energy= 0.252237

Optimized Geometry (XYZ coordinates in Å)

6	-1.728677	1.377081	1.060551
6	-0.396481	1.608938	0.625566
5	0.729680	0.528458	0.597434
7	-2.195891	0.099868	1.323850
6	-0.055349	2.926114	0.259813
1	0.957032	3.112735	-0.089216
6	-0.943459	3.987855	0.353363
1	-0.636550	4.991488	0.081280
6	-2.630847	2.451014	1.141010
1	-3.650039	2.259542	1.466567
6	-2.240548	3.735550	0.799950
1	-2.958471	4.546772	0.877814
1	-1.501154	-0.594647	1.556371
1	-3.021118	0.048204	1.901928

6	1.787751	0.535677	-0.558488
6	3.103075	0.078853	-0.361257
6	1.448033	0.997135	-1.843038
6	4.037837	0.090168	-1.391347
6	2.369456	0.988102	-2.884803
6	3.668600	0.538791	-2.657567
1	3.397758	-0.278510	0.621930
1	0.439546	1.360514	-2.021401
1	5.051570	-0.253312	-1.210462
1	2.079052	1.335460	-3.871355
1	4.393097	0.539436	-3.466341
6	0.865142	-0.529828	1.754841
6	0.519414	-0.188880	3.075680
6	1.339414	-1.832451	1.524074
6	0.659272	-1.096997	4.119508
6	1.456433	-2.755792	2.559652
6	1.123791	-2.385666	3.860302
1	0.139155	0.810332	3.276801
1	1.613936	-2.123914	0.513556
1	0.401948	-0.805650	5.133083
1	1.812839	-3.760387	2.354634
1	1.224737	-3.100250	4.671415

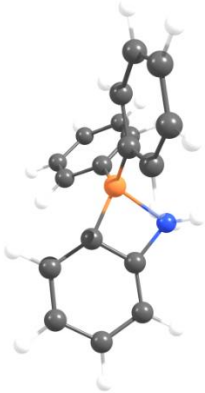

Figure S8: Computed structure of H/Ph (CLA)

Data for system: **H/Ph (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -775.1389427 A.U.
Zero-point correction= 0.297381 (Hartree/Particle)
Thermal correction to Energy= 0.313302
Thermal correction to Enthalpy= 0.314246
Thermal correction to Gibbs Free Energy= 0.252653

Optimized Geometry (XYZ coordinates in Å)

6	-1.383449	1.420055	0.915685
6	-0.174407	2.011845	0.590731
5	0.625343	0.601901	0.604597

7	-1.018511	0.005944	1.010505
6	-0.148468	3.394256	0.426001
1	0.767801	3.922738	0.179269
6	-1.341056	4.104340	0.590198
1	-1.343515	5.182956	0.464659
6	-2.587853	2.077975	1.093234
1	-3.510064	1.565938	1.350182
6	-2.539826	3.462769	0.918293
1	-3.444302	4.049678	1.039923
1	-1.125507	-0.404434	1.937211
1	-1.450233	-0.596274	0.311020
6	1.016170	-0.045378	-0.802089
6	1.221637	-1.428845	-0.928187
6	1.138102	0.728362	-1.962246
6	1.535386	-2.013654	-2.151521
6	1.463972	0.156724	-3.190950
6	1.660818	-1.217543	-3.288677
1	1.144155	-2.058670	-0.042615
1	0.968154	1.800927	-1.900540
1	1.687460	-3.086841	-2.219868
1	1.557770	0.782441	-4.073563
1	1.909619	-1.667517	-4.244891
6	1.557252	0.299273	1.874756
6	1.152239	0.688806	3.161969
6	2.795522	-0.345592	1.765340
6	1.927462	0.429698	4.287305
6	3.587563	-0.600750	2.884185
6	3.152886	-0.219896	4.149598
1	0.211964	1.227502	3.284627
1	3.149031	-0.650000	0.783851
1	1.584489	0.742095	5.269310
1	4.545281	-1.099156	2.766557
1	3.766360	-0.420144	5.022699

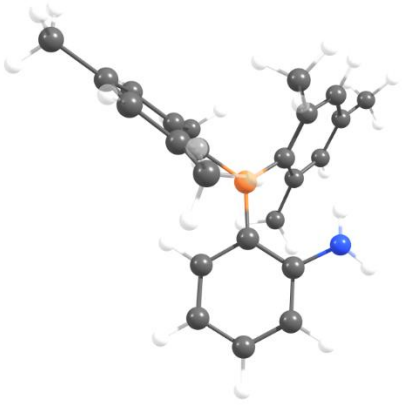

Figure S9: Computed structure of H/Mes (FLP)

Data for system: **H/Mes (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1011.007741 A.U.
Zero-point correction= 0.463111 (Hartree/Particle)

Thermal correction to Energy= 0.489724
Thermal correction to Enthalpy= 0.490668
Thermal correction to Gibbs Free Energy= 0.405621

Optimized Geometry (XYZ coordinates in Å)

6	-0.659076	2.651251	0.332661
6	0.052025	1.749574	1.169295
5	0.804644	0.478596	0.675960
7	-0.857847	2.392860	-1.009369
6	0.117271	2.055434	2.543580
1	0.642505	1.357869	3.192198
6	-0.441016	3.201352	3.088141
1	-0.354433	3.411608	4.148236
6	-1.240002	3.804772	0.888782
1	-1.789078	4.483518	0.241272
6	-1.125003	4.076221	2.241456
1	-1.578510	4.978506	2.641413
1	-1.118987	3.179955	-1.582605
1	-0.225827	1.741985	-1.453563
6	1.451108	0.373524	-0.767472
6	1.202793	-0.747222	-1.591474
6	0.263178	-1.852899	-1.164640
1	0.726233	-2.492872	-0.406999
1	-0.660641	-1.460510	-0.729465
1	-0.008328	-2.476246	-2.019865
6	1.827171	-0.853440	-2.834724
1	1.610949	-1.715552	-3.462620
6	2.726256	0.109055	-3.288152
6	3.432761	-0.049573	-4.609372
1	2.826355	-0.620120	-5.316891
1	3.660864	0.921198	-5.056215
1	4.380069	-0.583833	-4.481306
1	3.667130	1.977177	-2.810242
6	2.970242	1.212492	-2.472488
6	2.341482	1.367734	-1.237262
6	2.644550	2.617442	-0.439693
1	1.827883	3.342349	-0.523989
1	2.772164	2.416376	0.626897
1	3.555957	3.093320	-0.809089
6	0.972508	-0.738137	1.670111
6	-0.158170	-1.314524	2.290831
6	-1.560547	-0.781455	2.082145
1	-1.770040	0.051771	2.760592
1	-1.723910	-0.403158	1.069652
1	-2.296134	-1.566607	2.274346
6	-0.007477	-2.432654	3.112572
1	-0.891577	-2.879807	3.563177
6	1.241443	-2.990188	3.372342
6	1.390910	-4.168807	4.298955
1	0.469125	-4.753153	4.349045
1	2.199070	-4.828581	3.973072
1	1.627907	-3.836904	5.315338
1	3.341126	-2.832628	2.956370
6	2.355633	-2.411169	2.767011
6	2.239655	-1.313054	1.916596
6	3.498849	-0.768908	1.278485
1	3.560373	-1.046030	0.221151
1	3.543387	0.323142	1.325392
1	4.384283	-1.160495	1.784922

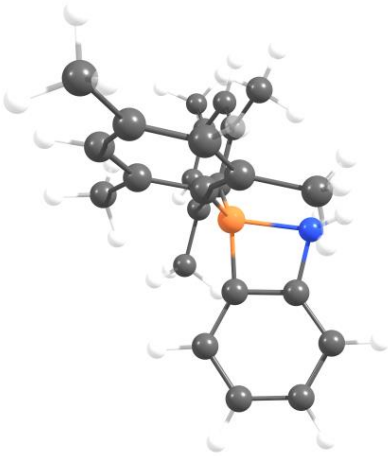

Figure S10: Computed structure of H/Mes (CLA)

Data for system: **H/Mes (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1010.986287 A.U.
Zero-point correction= 0.465125 (Hartree/Particle)
Thermal correction to Energy= 0.490492
Thermal correction to Enthalpy= 0.491436
Thermal correction to Gibbs Free Energy= 0.410125

Optimized Geometry (XYZ coordinates in Å)

6	-0.503516	3.111994	0.486365
6	0.105916	2.533482	1.585462
5	0.416331	1.138373	0.809505
7	-0.361670	2.074642	-0.532921
6	0.103459	3.248380	2.781062
1	0.549017	2.845933	3.687190
6	-0.490307	4.511723	2.800320
1	-0.500492	5.084280	3.722880
6	-1.107382	4.358189	0.454658
1	-1.573966	4.765010	-0.437373
6	-1.083876	5.063011	1.658897
1	-1.538000	6.046835	1.713828
1	-1.228497	1.792794	-0.981210
1	0.336144	2.289477	-1.244899
6	1.864972	0.806600	0.161945
6	1.941637	-0.215847	-0.814830
6	0.731594	-1.022301	-1.236767
1	0.456144	-1.757130	-0.474554
1	-0.152867	-0.397124	-1.393889
1	0.935723	-1.554972	-2.168904
6	3.155056	-0.529762	-1.429649
1	3.179029	-1.319863	-2.178250
6	4.333243	0.136799	-1.109176
6	5.644573	-0.242114	-1.747590

1	5.495782	-0.630200	-2.758472
1	6.319794	0.615333	-1.805404
1	6.151025	-1.021144	-1.167894
1	5.162856	1.702621	0.092805
6	4.258152	1.154709	-0.164080
6	3.058581	1.502190	0.463045
6	3.119917	2.639601	1.459131
1	2.521935	3.497381	1.139491
1	2.745238	2.346992	2.443698
1	4.152061	2.976055	1.582902
6	-0.426981	-0.108088	1.409962
6	-1.761265	-0.465386	1.122056
6	-2.645770	0.320940	0.178283
1	-2.646862	1.389969	0.418916
1	-2.353738	0.186144	-0.872044
1	-3.679770	-0.021996	0.254659
6	-2.349020	-1.581500	1.724109
1	-3.378086	-1.832397	1.473072
6	-1.668565	-2.371324	2.642970
6	-2.304904	-3.591927	3.255781
1	-3.395449	-3.527642	3.225921
1	-2.012390	-4.499990	2.717832
1	-1.998680	-3.716726	4.297795
1	0.172503	-2.555256	3.726824
6	-0.374595	-1.985247	2.977726
6	0.242321	-0.880961	2.389780
6	1.638062	-0.538017	2.862994
1	2.401702	-0.840318	2.140337
1	1.755663	0.538988	3.018004
1	1.848599	-1.036247	3.812571

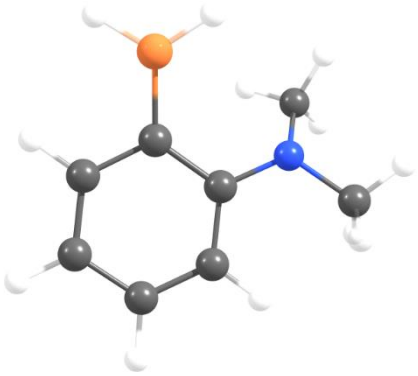

Figure S11: Computed structure of CH3/H (FLP)

Data for system: **CH3/H (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -391.6199788 A.U.
Zero-point correction= 0.187084 (Hartree/Particle)
Thermal correction to Energy= 0.196869
Thermal correction to Enthalpy= 0.197813
Thermal correction to Gibbs Free Energy= 0.152722

Optimized Geometry (XYZ coordinates in Å)

6	-1.428183	1.821766	0.349318
6	-0.118771	1.792103	0.915534
5	0.653316	0.508090	1.239135
7	-1.966145	0.689518	-0.245385
6	0.406053	2.994093	1.431059
1	1.412510	2.970512	1.840828
6	-0.324571	4.170730	1.478801
1	0.098883	5.075670	1.899677
6	-2.175517	3.012267	0.421796
1	-3.174429	3.058806	0.005150
6	-1.627847	4.157942	0.982222
1	-2.225628	5.064730	1.008146
6	-1.171655	-0.124623	-1.153750
6	-3.380680	0.654493	-0.548469
1	-3.645357	1.251699	-1.436179
1	-3.668879	-0.382135	-0.740387
1	-3.960387	1.013396	0.304121
1	-0.136019	0.213759	-1.158187
1	-1.191213	-1.180746	-0.866893
1	-1.562505	-0.033135	-2.177422
1	1.776980	0.594751	1.636916
1	0.148441	-0.570513	1.172820

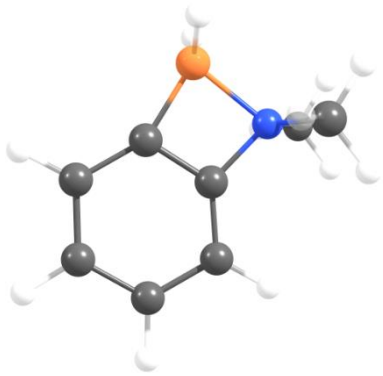

Figure S12: Computed structure of CH3/H (CLA)

Data for system: **CH3/H (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -391.6319865 A.U.
Zero-point correction= 0.188453 (Hartree/Particle)
Thermal correction to Energy= 0.197459
Thermal correction to Enthalpy= 0.198403
Thermal correction to Gibbs Free Energy= 0.155212

Optimized Geometry (XYZ coordinates in Å)

6	-1.456086	1.897809	0.573453
6	-0.130967	1.880350	0.974608
5	0.027637	0.332841	0.530048

7	-1.630811	0.525976	0.081476
6	0.390141	3.055399	1.510297
1	1.420073	3.123339	1.848186
6	-0.447150	4.170982	1.610099
1	-0.057246	5.095696	2.025459
6	-2.328635	2.968673	0.648289
1	-3.362009	2.922562	0.316446
6	-1.780757	4.134718	1.189277
1	-2.396050	5.023444	1.284619
6	-1.906447	0.444025	-1.362086
6	-2.592143	-0.267137	0.864603
1	-3.614336	0.085688	0.690401
1	-2.509294	-1.315039	0.568568
1	-2.341597	-0.170248	1.920648
1	-2.914073	0.812309	-1.582932
1	-1.167693	1.046315	-1.890171
1	-1.817350	-0.596983	-1.679898
1	0.655489	0.087448	-0.468126
1	0.082969	-0.505113	1.393523

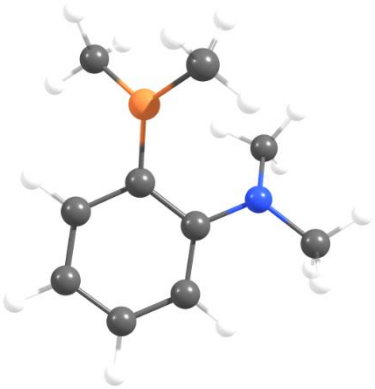

Figure S13: Computed structure of CH3/CH3 (FLP)

Data for system: **CH3/CH3 (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -470.2684034 A.U.
Zero-point correction= 0.243813 (Hartree/Particle)
Thermal correction to Energy= 0.257112
Thermal correction to Enthalpy= 0.258056
Thermal correction to Gibbs Free Energy= 0.204841

Optimized Geometry (XYZ coordinates in Å)

6	-1.282038	1.915645	0.379219
6	0.005620	1.950375	0.977570
5	0.960045	0.717281	1.115746
7	-1.675297	0.794406	-0.361883
6	0.377627	3.117497	1.659191
1	1.366755	3.162209	2.107996

6	-0.487321	4.193925	1.832759
1	-0.175236	5.070589	2.389751
6	-2.151924	3.003195	0.547038
1	-3.133433	2.995806	0.088033
6	-1.758813	4.120223	1.277553
1	-2.452474	4.948337	1.389728
6	0.410827	-0.730380	1.426694
6	2.526847	0.896536	1.027419
6	-0.767676	0.225862	-1.344658
6	-3.061754	0.671403	-0.754630
1	2.891072	1.924487	1.090496
1	3.066210	0.274275	1.748831
1	2.822852	0.519844	0.036495
1	0.679580	-0.952962	2.469026
1	0.919873	-1.496091	0.829011
1	-0.668560	-0.847130	1.320414
1	-3.343142	1.359495	-1.569325
1	-3.236031	-0.350565	-1.101717
1	-3.715026	0.854364	0.101004
1	-1.077110	0.497527	-2.365429
1	0.244781	0.604903	-1.198925
1	-0.742428	-0.867000	-1.269356

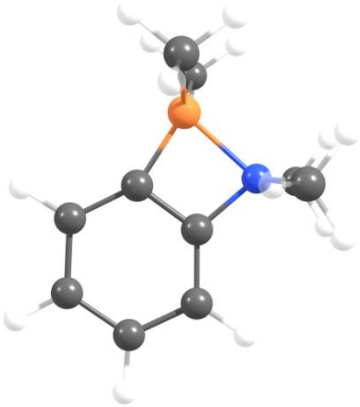

Figure S14: Computed structure of CH3/CH3 (CLA)

Data for system: **CH3/CH3 (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -470.2692425 A.U.
Zero-point correction= 0.244780 (Hartree/Particle)
Thermal correction to Energy= 0.257412
Thermal correction to Enthalpy= 0.258356
Thermal correction to Gibbs Free Energy= 0.207439

Optimized Geometry (XYZ coordinates in Å)

6	-1.327164	1.887195	0.593185
6	-0.015214	1.965448	1.029826
5	0.323189	0.435855	0.609652
7	-1.426527	0.515799	0.091102

6	0.408966	3.173812	1.577653
1	1.423401	3.310572	1.941568
6	-0.502088	4.231469	1.656385
1	-0.186019	5.179826	2.081074
6	-2.267778	2.901934	0.647974
1	-3.287165	2.786926	0.290087
6	-1.817936	4.103144	1.201167
1	-2.496310	4.946608	1.279044
6	0.491250	-0.654661	1.776169
6	1.255199	0.187163	-0.674002
6	-1.696882	0.437675	-1.352730
6	-2.381181	-0.315602	0.840394
1	1.171462	0.942011	-1.462706
1	2.300546	0.202291	-0.342546
1	1.091194	-0.798993	-1.126623
1	1.536303	-0.637407	2.108469
1	0.297286	-1.676633	1.426561
1	-0.118239	-0.478453	2.668533
1	-3.410892	-0.012695	0.618380
1	-2.241915	-1.361824	0.557492
1	-2.193101	-0.203411	1.906877
1	-2.728590	0.739458	-1.566904
1	-1.009965	1.096423	-1.881448
1	-1.542457	-0.590270	-1.689598

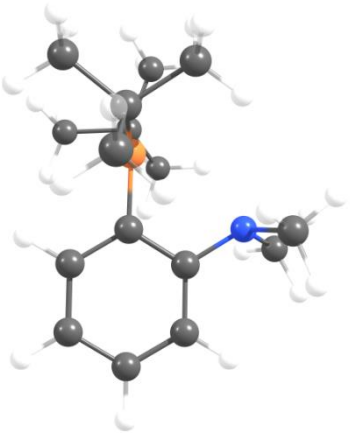

Figure S15: Computed structure of CH3/t-but (FLP)

Data for system: **CH3/t-but (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -706.096897326 A.U.
Zero-point correction= 0.415953 (Hartree/Particle)
Thermal correction to Energy= 0.436638
Thermal correction to Enthalpy= 0.437582
Thermal correction to Gibbs Free Energy= 0.369245

Optimized Geometry (XYZ coordinates in Å)

6	-1.562804	1.877532	0.334317
6	-0.359900	2.051486	1.028207
5	0.770504	0.945302	0.939639
7	-1.724554	0.644300	-0.403955
6	-0.198580	3.224008	1.778937
1	0.720602	3.379769	2.341225
6	-1.186897	4.204102	1.813847
1	-1.033500	5.110040	2.391715
6	-2.562030	2.851619	0.372809
1	-3.489983	2.698259	-0.171648
6	-2.371660	4.018565	1.106523
1	-3.147862	4.776750	1.131221
6	0.912040	-0.081834	2.171320
6	1.808087	1.068286	-0.275387
6	-2.204513	0.847784	-1.768112
6	-2.607221	-0.291031	0.289831
1	-3.647996	0.072073	0.335688
1	-2.599988	-1.250859	-0.236518
1	-2.255699	-0.453720	1.309726
1	-3.270326	1.126453	-1.812331
1	-1.620306	1.631036	-2.253418
1	-2.080176	-0.082570	-2.331163
6	2.584907	-0.196434	-0.668851
1	3.157285	-0.626590	0.156142
1	1.911106	-0.969273	-1.052321
1	3.297686	0.043515	-1.468073
6	2.814315	2.136683	0.226748
1	2.317102	3.089403	0.438078
1	3.353256	1.821297	1.125256
1	3.559176	2.321823	-0.557095
6	1.165807	1.615431	-1.559451
1	1.944360	1.847422	-2.297248
1	0.494670	0.873343	-2.000405
1	0.592607	2.529145	-1.374294
6	2.309575	-0.032104	2.819883
1	2.357352	-0.757537	3.641949
1	3.114411	-0.272440	2.122195
1	2.517646	0.955807	3.246747
6	0.656505	-1.512351	1.648211
1	-0.272998	-1.578493	1.072486
1	1.467502	-1.865498	1.008586
1	0.574184	-2.204308	2.495773
6	-0.100177	0.208316	3.293259
1	-1.134167	0.188455	2.937439
1	-0.002765	-0.537178	4.092067
1	0.062097	1.196797	3.734622

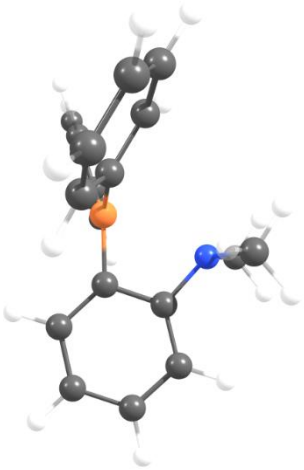

Figure S16: Computed structure of CH3/Ph (FLP)

Data for system: **CH3/Ph (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -853.7380715 A.U.
Zero-point correction= 0.352791 (Hartree/Particle)
Thermal correction to Energy= 0.372162
Thermal correction to Enthalpy= 0.373106
Thermal correction to Gibbs Free Energy= 0.303509

Optimized Geometry (XYZ coordinates in Å)

6	-3.308183	4.455703	-1.622921
6	-1.915332	4.433810	-1.703229
5	-1.365918	3.071735	-1.115362
7	-3.866603	3.262641	-1.026911
6	-1.260548	5.528238	-2.271102
1	-0.177448	5.532405	-2.362415
6	-1.995667	6.620955	-2.730714
1	-1.483351	7.471521	-3.169582
6	-4.055984	5.535997	-2.083235
1	-5.140689	5.529747	-2.012951
6	-3.386766	6.625029	-2.639173
1	-3.950814	7.477220	-3.004961
6	-4.779853	2.542996	-1.903776
6	-4.445763	3.509952	0.288984
1	-5.357014	4.128154	0.239949
1	-4.698097	2.551915	0.753446
1	-3.708347	4.013304	0.918801
1	-5.709372	3.099166	-2.108159
1	-4.281622	2.330367	-2.852405
1	-5.047239	1.592238	-1.433909
6	-0.986453	1.909913	-2.097698
6	-0.170182	0.835240	-1.707691
6	-1.429863	1.934736	-3.431546
6	0.171051	-0.177835	-2.598916
6	-1.107800	0.919071	-4.324855
6	-0.306059	-0.141497	-3.906791

1	0.216379	0.803289	-0.692966
1	-2.032963	2.774261	-3.769968
1	0.809463	-0.994259	-2.275872
1	-1.469932	0.956654	-5.347575
1	-0.044977	-0.932846	-4.602963
6	-1.148803	2.968432	0.436232
6	-0.753471	4.091631	1.178544
6	-1.427456	1.786655	1.142794
6	-0.606574	4.032522	2.561912
6	-1.309615	1.726491	2.527685
6	-0.888487	2.848643	3.238942
1	-0.566471	5.029091	0.659683
1	-1.766746	0.910771	0.595072
1	-0.287500	4.911427	3.113596
1	-1.544863	0.806622	3.054305
1	-0.788944	2.802379	4.319086

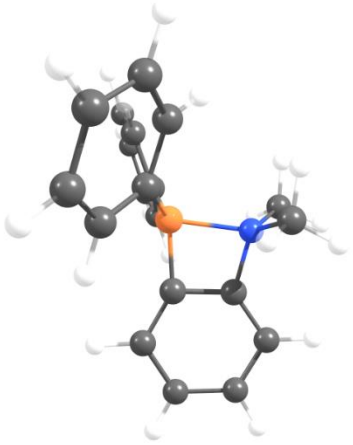

Figure S17: Computed structure of CH3/Ph (CLA)

Data for system: **CH3/Ph (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -853.7417688 A.U.
Zero-point correction= 0.354108 (Hartree/Particle)
Thermal correction to Energy= 0.372720
Thermal correction to Enthalpy= 0.373664
Thermal correction to Gibbs Free Energy= 0.307163

Optimized Geometry (XYZ coordinates in Å)

6	-3.153485	4.710071	-1.695838
6	-1.795134	4.968014	-1.737518
5	-1.377866	3.496306	-1.216084
7	-3.223325	3.355563	-1.145505
6	-1.380777	6.208978	-2.215033
1	-0.328400	6.469078	-2.287726
6	-2.355102	7.128138	-2.615773
1	-2.052121	8.102024	-2.988475
6	-4.155704	5.582344	-2.086722

1	-5.211798	5.332608	-2.039294
6	-3.718459	6.823014	-2.556785
1	-4.445551	7.559965	-2.882184
6	-3.880912	2.372495	-2.021631
6	-3.835193	3.343741	0.196358
1	-4.896070	3.608881	0.124683
1	-3.734427	2.347374	0.631345
1	-3.314783	4.060393	0.831397
1	-4.960669	2.556184	-2.059018
1	-3.459231	2.438858	-3.023125
1	-3.694376	1.370733	-1.626701
6	-0.810810	2.497817	-2.341666
6	-0.079262	1.341497	-2.034557
6	-1.007366	2.773426	-3.706421
6	0.401923	0.489397	-3.027186
6	-0.534980	1.929726	-4.707156
6	0.169449	0.776729	-4.368317
1	0.142572	1.109836	-0.997432
1	-1.538282	3.679988	-3.991633
1	0.966905	-0.396154	-2.751331
1	-0.706661	2.175963	-5.750909
1	0.545042	0.116340	-5.144019
6	-0.824709	3.345435	0.274339
6	-0.184057	4.415938	0.910828
6	-0.969967	2.159911	1.014457
6	0.308342	4.309157	2.210554
6	-0.495141	2.043815	2.317328
6	0.152686	3.121397	2.918603
1	-0.074662	5.356591	0.375729
1	-1.472375	1.306789	0.559431
1	0.806413	5.155863	2.673564
1	-0.626483	1.114578	2.863946
1	0.528966	3.035229	3.933268

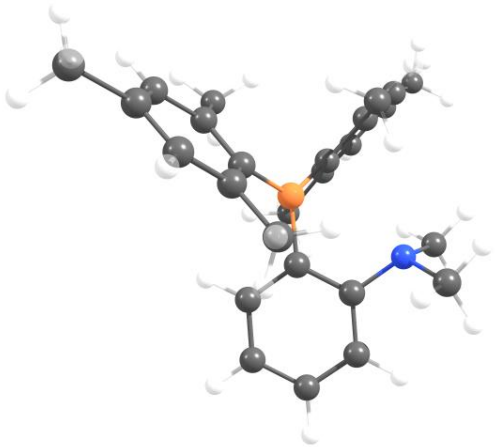

Figure S18: Computed structure of CH3/Mes (FLP)

Data for system: **CH3/Mes (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1089.59467909 A.U.
Zero-point correction= 0.519733 (Hartree/Particle)
Thermal correction to Energy= 0.548899
Thermal correction to Enthalpy= 0.549844
Thermal correction to Gibbs Free Energy= 0.459373

Optimized Geometry (XYZ coordinates in Å)

6	-1.770754	1.947641	-0.048666
6	-0.776003	2.010406	0.940260
5	0.372538	0.930171	1.019948
7	-1.771437	0.809013	-0.934055
6	-0.824361	3.063212	1.862992
1	-0.085852	3.099254	2.661487
6	-1.799603	4.053929	1.784042
1	-1.814555	4.864261	2.505953
6	-2.757655	2.931239	-0.122245
1	-3.527704	2.866803	-0.886224
6	-2.768143	3.986733	0.786410
1	-3.540163	4.747289	0.722755
6	-1.233961	1.122044	-2.255766
6	-3.072632	0.163876	-1.054993
1	-3.798346	0.746199	-1.647585
1	-2.940904	-0.803150	-1.550987
1	-3.497226	-0.007210	-0.062975
1	-1.914776	1.767158	-2.837672
1	-0.268685	1.620998	-2.158514
1	-1.079828	0.188846	-2.807613
6	0.620429	0.179594	2.381936
6	1.924264	0.011075	2.907646
1	3.076576	1.532847	1.857749
1	3.358583	-0.104001	1.290556
6	3.163317	0.493843	2.185620
1	4.034088	0.422132	2.841405
1	3.110022	-0.730794	4.534041
6	2.102720	-0.624403	4.136623
6	1.031456	-1.141109	4.860917
6	1.247304	-1.809272	6.193505
1	1.197971	-1.077269	7.006597
1	2.227783	-2.289211	6.241882
1	0.483077	-2.566257	6.385457
6	-0.246578	-1.009244	4.322861
1	-1.094121	-1.432105	4.858557
1	-2.517998	-1.006901	3.125083
6	-1.889697	-0.283930	2.599201
1	-1.937418	-0.506440	1.529075
1	-2.321848	0.711398	2.741586
6	-0.468618	-0.351625	3.114462
6	1.287626	0.700080	-0.242390
6	1.368803	-0.579502	-0.830072
1	-0.493881	-1.487475	-0.268105
1	0.863909	-1.960904	0.759683
6	0.574228	-1.735486	-0.271126
1	0.715891	-2.636267	-0.873049
1	2.197055	-1.764222	-2.415418
6	2.151687	-0.773364	-1.966914
6	2.882456	0.267130	-2.540132

6	3.711914	0.037720	-3.777338
1	3.091943	0.088359	-4.678721
1	4.183724	-0.948161	-3.760124
1	4.496948	0.791438	-3.873609
6	2.800965	1.526792	-1.951307
1	3.366686	2.351610	-2.380555
1	2.732843	3.786121	-0.676957
6	1.923946	3.168053	-0.280040
1	1.986274	3.196030	0.812675
1	0.972055	3.638990	-0.549349
6	2.005199	1.760615	-0.828425

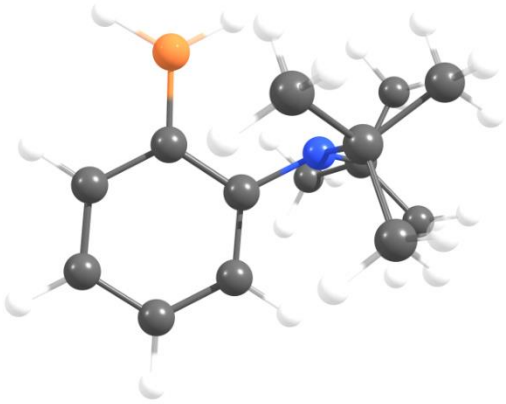

Figure S19: Computed structure of t-but/H (FLP)

Data for system: **t-but/H (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -627.4618345 A.U.
Zero-point correction= 0.357242 (Hartree/Particle)
Thermal correction to Energy= 0.374433
Thermal correction to Enthalpy= 0.375378
Thermal correction to Gibbs Free Energy= 0.314923

Optimized Geometry (XYZ coordinates in Å)

6	-2.981814	-0.609513	-2.741512
6	-3.213340	-0.885669	-1.371247
5	-2.291438	-0.380281	-0.237769
7	-1.794285	0.094734	-3.129489
6	-4.361342	-1.620244	-1.020782
1	-4.528328	-1.849099	0.028455
6	-5.282808	-2.045246	-1.969409
1	-6.165558	-2.602081	-1.672867
6	-3.913086	-1.045191	-3.690336
1	-3.742652	-0.823856	-4.739193
6	-5.054569	-1.747508	-3.309993
1	-5.762963	-2.069399	-4.067721
6	-0.716826	-0.809885	-3.629352
6	-1.988786	1.497443	-3.613563

6	-1.044788	-1.509655	-4.965723
1	-0.189892	-2.116868	-5.280656
1	-1.900631	-2.180634	-4.859566
1	-1.259377	-0.795242	-5.763329
6	-0.483530	-1.913551	-2.581291
1	-1.354396	-2.561746	-2.463289
1	0.359156	-2.536802	-2.894364
1	-0.242599	-1.470156	-1.609131
6	0.621295	-0.077170	-3.779969
1	1.392910	-0.814611	-4.017925
1	0.614981	0.654622	-4.589770
1	0.899796	0.420796	-2.848374
6	-3.317294	2.039741	-3.053249
1	-3.338059	1.963511	-1.962298
1	-3.403503	3.094715	-3.324813
1	-4.189006	1.517007	-3.450219
6	-0.900762	2.431305	-3.040342
1	-0.760170	2.223374	-1.976516
1	0.059646	2.341299	-3.544791
1	-1.223190	3.471258	-3.150463
6	-2.033122	1.651730	-5.143889
1	-1.090754	1.365796	-5.616619
1	-2.836097	1.051020	-5.581932
1	-2.222556	2.699473	-5.399718
1	-1.440392	0.431787	-0.422802
1	-2.470394	-0.796581	0.868666

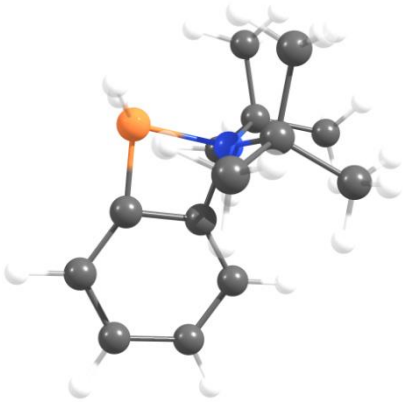

Figure S20: Computed structure of t-but/H (CLA)

Data for system: t-but/H (CLA)

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -627.4618345 A.U.
Zero-point correction= 0.360004 (Hartree/Particle)
Thermal correction to Energy= 0.376267
Thermal correction to Enthalpy= 0.377211
Thermal correction to Gibbs Free Energy= 0.319197

Optimized Geometry (XYZ coordinates in Å)

6	-3.009435	-0.660262	-2.626068

6	-3.316635	-0.963173	-1.308999
5	-2.045406	-0.154259	-0.752298
7	-1.708215	0.029321	-2.488770
6	-4.482349	-1.676520	-1.048325
1	-4.772391	-1.943680	-0.036195
6	-5.293941	-2.046412	-2.124396
1	-6.206968	-2.605688	-1.942643
6	-3.796438	-0.985853	-3.720898
1	-3.553662	-0.700787	-4.739917
6	-4.964419	-1.699367	-3.436976
1	-5.625513	-1.985042	-4.248854
6	-0.566994	-0.898683	-2.979213
6	-1.731246	1.513697	-2.921503
6	-0.561592	-1.143173	-4.499545
1	0.142387	-1.956923	-4.694650
1	-1.538432	-1.476693	-4.855418
1	-0.233793	-0.292673	-5.090658
6	-0.738526	-2.301720	-2.357621
1	-1.645802	-2.792243	-2.715878
1	0.116091	-2.902768	-2.678194
1	-0.754363	-2.283384	-1.271017
6	0.788605	-0.340232	-2.544801
1	1.544437	-1.118770	-2.678866
1	1.095741	0.513087	-3.152845
1	0.776112	-0.051451	-1.491053
6	-3.144846	2.075044	-2.672461
1	-3.496934	1.874459	-1.661314
1	-3.102798	3.157949	-2.813778
1	-3.869684	1.671140	-3.381599
6	-0.738221	2.341800	-2.089897
1	-0.875040	2.175046	-1.021729
1	0.300503	2.144665	-2.348285
1	-0.925165	3.399355	-2.297299
6	-1.427846	1.743217	-4.406427
1	-0.371237	1.608354	-4.644070
1	-2.030053	1.102473	-5.055675
1	-1.680041	2.781626	-4.640084
1	-2.307855	0.920280	-0.286888
1	-1.133109	-0.686019	-0.182618

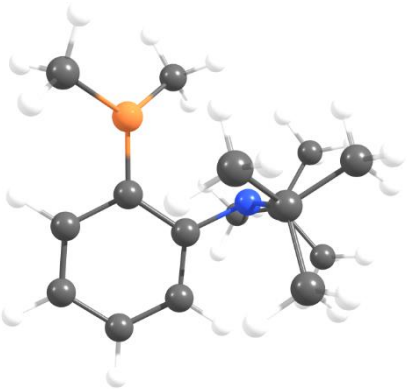

Figure S21: Computed structure of t-but/CH3 (FLP)

Data for system: **t-but/CH3 (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -706.101628954 A.U.
Zero-point correction= 0.414557 (Hartree/Particle)
Thermal correction to Energy= 0.434978
Thermal correction to Enthalpy= 0.435923
Thermal correction to Gibbs Free Energy= 0.369060

Optimized Geometry (XYZ coordinates in Å)

6	-3.024410	-0.538635	-2.693488
6	-3.275314	-0.920780	-1.360985
5	-2.307820	-0.622185	-0.155331
7	-1.801556	0.158779	-3.010859
6	-4.448988	-1.642939	-1.085740
1	-4.636996	-1.972109	-0.066163
6	-5.383262	-1.938822	-2.070848
1	-6.292685	-2.476358	-1.822060
6	-3.947860	-0.883838	-3.689125
1	-3.739689	-0.612341	-4.719085
6	-5.125891	-1.557237	-3.383894
1	-5.831295	-1.796152	-4.173830
6	-0.723390	-0.772958	-3.474935
6	-1.973821	1.533846	-3.594252
6	-1.043313	-1.509116	-4.792977
1	-0.200023	-2.152426	-5.064370
1	-1.922572	-2.148247	-4.682073
1	-1.216913	-0.820882	-5.622161
6	-0.507580	-1.853959	-2.399257
1	-1.385711	-2.488163	-2.263520
1	0.326108	-2.496264	-2.697552
1	-0.249824	-1.397025	-1.437248
6	0.626074	-0.060268	-3.625525
1	1.394254	-0.813834	-3.820329
1	0.647352	0.642450	-4.459836
1	0.892637	0.468307	-2.706688
6	-3.324737	2.111609	-3.127615
1	-3.437253	2.025847	-2.043715
1	-3.361535	3.170529	-3.395134
1	-4.178215	1.617785	-3.593767
6	-0.901031	2.498127	-3.041829
1	-0.810416	2.384552	-1.959967
1	0.080620	2.356014	-3.489950
1	-1.201396	3.528400	-3.255297
6	-1.949721	1.620821	-5.132474
1	-0.986765	1.324056	-5.553467
1	-2.730664	1.007775	-5.589995
1	-2.128582	2.658904	-5.431691
6	-1.657548	0.783625	0.129835
1	-1.546081	0.969487	1.203449
1	-0.642511	0.765394	-0.291232
1	-2.171776	1.627612	-0.333333
6	-2.052011	-1.773804	0.896718
1	-2.773088	-1.630413	1.716119
1	-2.198894	-2.786244	0.512083
1	-1.063338	-1.701344	1.360925

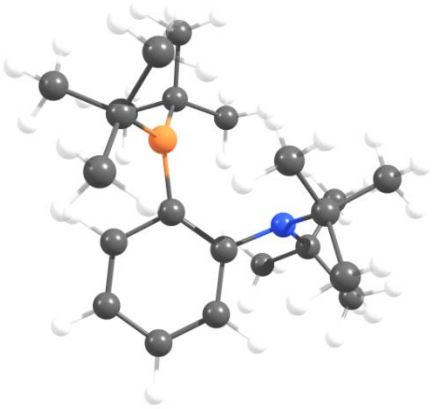

Figure S22: Computed structure of t-but/t-but (FLP)

Data for system: **t-but/t-but (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -941.917215084 A.U.
Zero-point correction= 0.588253 (Hartree/Particle)
Thermal correction to Energy= 0.615741
Thermal correction to Enthalpy= 0.616686
Thermal correction to Gibbs Free Energy= 0.536269

Optimized Geometry (XYZ coordinates in Å)

6	-3.714673	-0.862953	0.627779
6	-3.101449	-1.260293	1.843195
5	-1.812669	-2.160125	2.148447
7	-3.044731	-0.925655	-0.656050
6	-3.766310	-0.912376	3.036336
1	-3.295245	-1.165227	3.985106
6	-5.000701	-0.278747	3.074379
1	-5.455027	-0.018432	4.024828
6	-5.019209	-0.343183	0.682707
1	-5.527217	-0.136137	-0.252168
6	-5.659293	-0.037418	1.875543
1	-6.655306	0.393754	1.863014
6	-2.092023	-3.574951	2.912588
6	-0.348394	-1.510468	2.028809
6	0.877471	-2.436028	2.056758
6	-0.271588	-0.560071	3.254767
6	-0.205917	-0.629306	0.783600
6	-1.403639	-4.775322	2.223169
6	-1.521681	-3.487043	4.350638
6	-3.577515	-3.960454	3.074815
1	-0.437457	-3.360694	4.373171
1	-1.755902	-4.417540	4.882463
1	-1.474858	-5.651278	2.880027
1	-0.347140	-4.608019	2.014080
1	-1.896934	-5.038773	1.284065
1	-4.105991	-3.298747	3.764185
1	-4.131858	-3.944229	2.131898
1	-3.643752	-4.977717	3.479709

1	-0.256782	-1.218037	-0.137611
1	0.758945	-0.105023	0.802702
1	1.789475	-1.825933	2.058847
1	0.920289	-3.083823	2.934613
1	0.917874	-3.070720	1.165102
1	-0.301360	-1.094174	4.208734
1	0.676012	-0.008933	3.214678
1	-1.003543	0.112419	0.735014
1	-1.967262	-2.667693	4.925531
1	-1.084320	0.173271	3.245293
6	-3.229735	-2.228403	-1.367374
6	-3.009148	0.377638	-1.421789
6	-4.703599	-2.553255	-1.681568
1	-4.776182	-3.550395	-2.127676
1	-5.304066	-2.552337	-0.767879
1	-5.141517	-1.841214	-2.384240
6	-2.696129	-3.336619	-0.452611
1	-3.312279	-3.450155	0.437782
1	-2.698698	-4.296358	-0.978590
1	-1.661576	-3.118484	-0.155221
6	-2.409597	-2.345628	-2.658875
1	-1.344625	-2.199138	-2.460567
1	-2.542022	-3.359159	-3.048028
1	-2.724002	-1.658632	-3.444242
6	-3.123044	1.578392	-0.455510
1	-2.491150	1.452656	0.426874
1	-2.791403	2.474593	-0.985943
1	-4.141580	1.755473	-0.110904
6	-1.642125	0.567803	-2.119052
1	-0.829298	0.534011	-1.393057
1	-1.439859	-0.161356	-2.898456
1	-1.627914	1.553474	-2.594168
6	-4.106264	0.563350	-2.492396
1	-4.001072	1.561642	-2.929474
1	-4.027733	-0.155944	-3.309462
1	-5.113681	0.496064	-2.076269

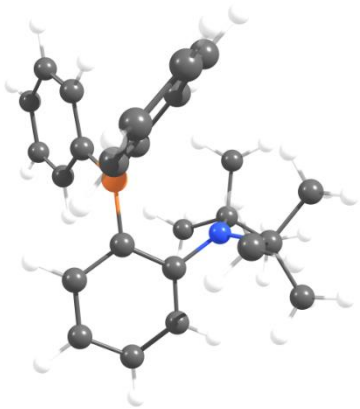

Figure S23: Computed structure of t-but/Ph (FLP)

Data for system: **t-but/Ph (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1089.57080274 A.U.
Zero-point correction= 0.524667 (Hartree/Particle)
Thermal correction to Energy= 0.550974
Thermal correction to Enthalpy= 0.551918
Thermal correction to Gibbs Free Energy= 0.469968

Optimized Geometry (XYZ coordinates in Å)

6	-2.952359	-0.649115	-2.689471
6	-3.266247	-0.650591	-1.316599
5	-2.346202	0.070250	-0.258512
7	-1.768118	0.046958	-3.126881
6	-4.435153	-1.300591	-0.892081
1	-4.697246	-1.285548	0.164254
6	-5.267391	-1.963111	-1.789481
1	-6.156818	-2.474663	-1.435599
6	-3.824584	-1.270490	-3.591088
1	-3.621585	-1.204995	-4.654727
6	-4.963912	-1.936018	-3.146904
1	-5.623147	-2.414839	-3.864360
6	-0.718367	-0.829872	-3.744187
6	-1.980738	1.465065	-3.590025
6	-1.047618	-1.394852	-5.148327
1	-0.146507	-1.860281	-5.560784
1	-1.806784	-2.177962	-5.083498
1	-1.384732	-0.641964	-5.859087
6	-0.484701	-2.054784	-2.842476
1	-1.411800	-2.589665	-2.622193
1	0.184624	-2.746117	-3.363963
1	-0.012162	-1.768073	-1.903537
6	0.636485	-0.107255	-3.793849
1	1.399330	-0.826944	-4.105228
1	0.669279	0.725238	-4.498471
1	0.901744	0.254701	-2.796878
6	-3.387669	1.958521	-3.208487
1	-3.544428	1.932011	-2.129872
1	-3.481093	2.998930	-3.531490
1	-4.177426	1.378351	-3.690653
6	-1.003643	2.407511	-2.862279
1	-1.144690	2.309580	-1.780590
1	0.041468	2.209870	-3.095069
1	-1.216053	3.446386	-3.135851
6	-1.872878	1.672128	-5.112333
1	-0.896707	1.410339	-5.521293
1	-2.638087	1.091815	-5.637315
1	-2.047972	2.728930	-5.336382
6	-0.960889	-0.566555	0.108879
6	-0.925089	-1.910953	0.507135
6	0.254724	0.130183	0.045139
6	0.273790	-2.536172	0.836579
6	1.462058	-0.500126	0.336052
6	1.472942	-1.834389	0.737627
1	-1.850632	-2.481855	0.536976
1	0.260192	1.172840	-0.264637
1	0.276477	-3.576178	1.147784
1	2.394396	0.050211	0.253403
1	2.412728	-2.324920	0.970943
6	-2.886244	1.297654	0.554516
6	-4.185587	1.800015	0.351052

6	-2.107048	1.910860	1.552632
6	-4.678273	2.867339	1.092955
6	-2.587623	2.986139	2.292203
6	-3.874744	3.466311	2.061217
1	-4.819075	1.336611	-0.401055
1	-1.112454	1.526893	1.758765
1	-5.684634	3.234232	0.917916
1	-1.965083	3.444469	3.054084
1	-4.254477	4.302755	2.640290

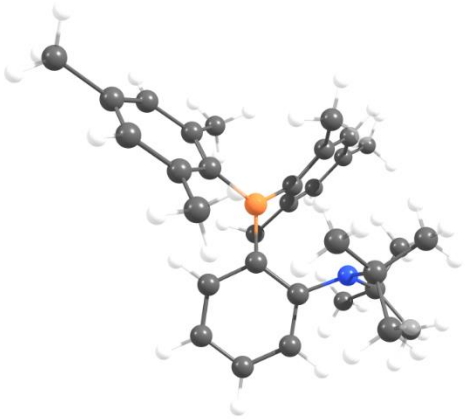

Figure S24: Computed structure of t-but/Mes (FLP)

Data for system: **t-but/Mes (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1325.41805010 A.U.
Zero-point correction= 0.692601 (Hartree/Particle)
Thermal correction to Energy= 0.728396
Thermal correction to Enthalpy= 0.729340
Thermal correction to Gibbs Free Energy= 0.628053

Optimized Geometry (XYZ coordinates in Å)

6	-3.581031	-0.232834	-2.594189
6	-3.704446	-0.552348	-1.214339
5	-2.743606	-0.122474	-0.023855
7	-2.426078	0.448709	-3.132122
6	-4.874852	-1.222299	-0.802026
1	-4.974394	-1.479166	0.250290
6	-5.901004	-1.560799	-1.673394
1	-6.791590	-2.059830	-1.305294
6	-4.605886	-0.629533	-3.467966
1	-4.493700	-0.409403	-4.524915
6	-5.758585	-1.266298	-3.025034
1	-6.533920	-1.537149	-3.735193
6	-1.384943	-0.489213	-3.662309
6	-2.678368	1.763783	-3.831525
6	-1.785481	-1.267373	-4.936527
1	-0.995268	-1.986951	-5.175568
1	-2.703869	-1.836780	-4.771056

1	-1.922386	-0.629679	-5.808926
6	-1.113801	-1.558079	-2.598337
1	-1.955572	-2.243741	-2.509728
1	-0.232049	-2.142336	-2.878363
1	-0.930229	-1.102578	-1.620372
6	-0.052595	0.229022	-3.911524
1	0.717454	-0.521658	-4.111489
1	-0.079924	0.896980	-4.773364
1	0.241581	0.805777	-3.031001
6	-4.017097	2.371137	-3.380392
1	-4.022850	2.508329	-2.300750
1	-4.112092	3.357992	-3.840460
1	-4.887126	1.782417	-3.672224
6	-1.613602	2.794679	-3.396688
1	-1.481052	2.750187	-2.314860
1	-0.647066	2.647751	-3.876541
1	-1.953188	3.800834	-3.663914
6	-2.716205	1.717334	-5.371710
1	-1.761380	1.428575	-5.813589
1	-3.490462	1.041939	-5.747045
1	-2.948320	2.721570	-5.740493
6	-2.187581	1.353946	-0.028785
6	-0.817029	1.660456	0.041504
6	0.243061	0.584433	0.094606
1	0.624374	0.345068	-0.903906
1	-0.140463	-0.341150	0.533256
1	1.094311	0.914907	0.695875
6	-0.401653	2.994839	0.091894
1	0.663439	3.214527	0.142572
6	-1.312630	4.046297	0.094343
1	-1.516190	6.106826	0.705974
6	-0.851224	5.480231	0.105895
1	0.160440	5.568375	0.509029
1	-0.840592	5.890844	-0.909498
1	-3.403127	4.538508	0.129482
6	-2.673249	3.732552	0.077423
6	-3.121741	2.415467	0.018163
6	-4.612246	2.153227	0.123595
1	-5.032303	1.720630	-0.787615
1	-4.839929	1.443007	0.927453
1	-5.148243	3.080672	0.339766
6	-2.563972	-1.040080	1.269788
6	-2.533723	-0.459751	2.576080
6	-2.557943	1.026923	2.875985
1	-2.624645	1.175210	3.955811
1	-3.404710	1.542174	2.422574
1	-1.655543	1.530932	2.522853
6	-2.485671	-1.274203	3.709855
1	-2.490732	-0.803266	4.690122
6	-2.425862	-2.659969	3.636176
1	-1.298174	-3.621686	5.195844
6	-2.339883	-3.505634	4.878601
1	-2.886649	-3.048605	5.706942
1	-2.745793	-4.505192	4.706004
1	-2.348082	-4.312148	2.279358
6	-2.413510	-3.230184	2.370041
6	-2.479594	-2.462341	1.207036
6	-2.358500	-3.247268	-0.079345
1	-2.516203	-4.310187	0.116181
1	-3.069181	-2.935471	-0.841629

1 -1.352357 -3.139900 -0.496436

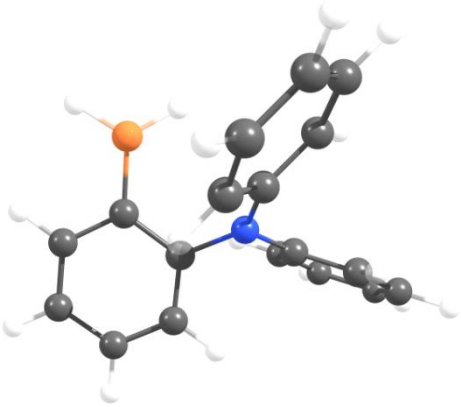

Figure S25: Computed structure of Ph/H (FLP)

Data for system: **Ph/H (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -775.1003833 A.U.
Zero-point correction= 0.292503 (Hartree/Particle)
Thermal correction to Energy= 0.308734
Thermal correction to Enthalpy= 0.309679
Thermal correction to Gibbs Free Energy= 0.247692

Optimized Geometry (XYZ coordinates in Å)

6	-2.854175	3.282104	1.875624
6	-2.467143	4.430243	2.575550
7	-1.988143	2.159669	1.842961
6	-3.312137	5.531822	2.632283
1	-2.998995	6.415553	3.179016
6	-4.542795	5.513213	1.979676
1	-5.196383	6.377975	2.018029
6	-4.094254	3.259214	1.228870
1	-4.397070	2.367887	0.689251
6	-4.924503	4.373829	1.276060
1	-5.883465	4.343597	0.768588
6	-1.396208	1.717578	3.051719
6	-0.055157	1.264587	3.070779
6	0.446689	0.765760	4.285698
1	1.468221	0.395446	4.303799
1	0.114186	0.391530	6.381933
6	-0.304888	0.765622	5.454177
6	-1.610523	1.251004	5.413824
1	-2.219335	1.249981	6.312942
1	-3.186930	2.061113	4.189409
6	-2.160169	1.711529	4.222493
6	-1.914389	1.357658	0.677229
6	-1.843006	-0.036736	0.770028
1	-1.861131	-0.509658	1.746157
6	-1.743311	-0.808779	-0.383392
1	-1.684366	-1.888885	-0.293830

1	-1.664249	-0.816977	-2.536224
6	-1.737386	-0.211014	-1.639791
6	-1.826657	1.176795	-1.731575
1	-1.817106	1.659242	-2.703822
1	-1.953055	3.040647	-0.659733
6	-1.906707	1.959013	-0.587165
5	0.917448	1.411158	1.879280
1	-1.501488	4.445030	3.071019
1	0.681236	2.125441	0.957489
1	1.966512	0.842281	1.927633

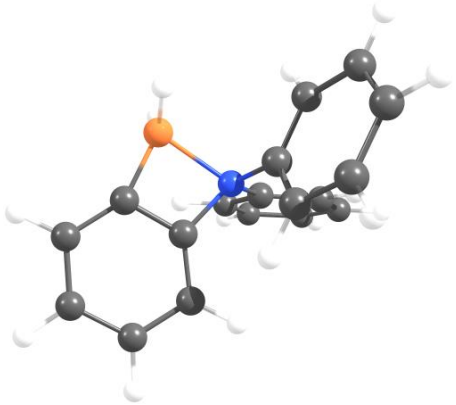

Figure S26: Computed structure of Ph/H (CLA)

Data for system: **Ph/H (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -775.0920741 A.U.
Zero-point correction= 0.293748 (Hartree/Particle)
Thermal correction to Energy= 0.309209
Thermal correction to Enthalpy= 0.310153
Thermal correction to Gibbs Free Energy= 0.250311

Optimized Geometry (XYZ coordinates in Å)

6	-0.767494	3.445047	1.066653
6	0.489059	3.915571	1.454116
7	-1.159501	2.100190	1.495105
6	0.888860	5.193999	1.090828
1	1.868577	5.549666	1.392110
6	0.043760	6.015025	0.345490
1	0.361333	7.012474	0.061002
6	-1.624686	4.264938	0.337894
1	-2.608185	3.914182	0.049499
6	-1.210207	5.546612	-0.023817
1	-1.883214	6.178055	-0.594521
6	-1.034584	1.913312	2.951519
6	-0.102260	0.900095	3.073738
6	0.255007	0.501665	4.360358
1	0.982491	-0.286263	4.530596
1	-0.064619	0.853751	6.457477

6	-0.332849	1.151323	5.448142
6	-1.247882	2.195603	5.274014
1	-1.668123	2.690524	6.143371
1	-2.302000	3.441360	3.832644
6	-1.617038	2.614154	3.995104
6	-2.382024	1.604758	0.877647
6	-3.553246	1.413365	1.597177
1	-3.581943	1.619674	2.660342
6	-4.688169	0.931933	0.941856
1	-5.601262	0.777014	1.507019
1	-5.538488	0.280629	-0.921687
6	-4.653157	0.653619	-0.417901
6	-3.469232	0.846340	-1.131937
1	-3.427968	0.619070	-2.191959
1	-1.399398	1.451777	-1.022163
6	-2.333877	1.313274	-0.486730
5	0.121020	0.763471	1.493242
1	1.141395	3.277936	2.039921
1	-0.371381	-0.163394	0.914845
1	1.106877	1.238805	1.001711

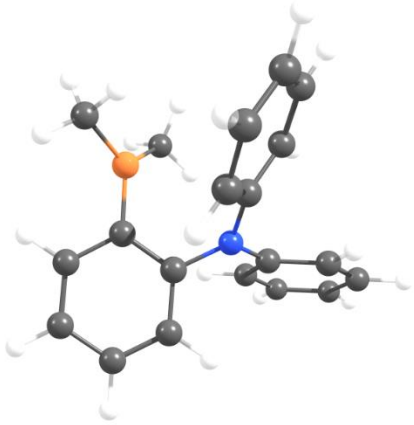

Figure S27: Computed structure of Ph/CH3 (FLP)

Data for system: **Ph/CH3 (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -853.752893577 A.U.
Zero-point correction= 0.349397 (Hartree/Particle)
Thermal correction to Energy= 0.368979
Thermal correction to Enthalpy= 0.369923
Thermal correction to Gibbs Free Energy= 0.300563

Optimized Geometry (XYZ coordinates in Å)

6	-1.476717	4.034539	1.416712
6	-0.469311	4.806285	2.009127
7	-1.534344	2.643561	1.653805
6	-0.418338	6.177939	1.788683
1	0.368749	6.761228	2.255983

6	-1.354128	6.799823	0.966552
1	-1.306662	7.869080	0.791397
6	-2.424893	4.662968	0.599344
1	-3.212445	4.070147	0.145783
6	-2.353165	6.031861	0.372468
1	-3.095186	6.503248	-0.264254
6	-1.167764	2.128223	2.930184
6	-0.296104	1.026711	3.008039
6	-0.036728	0.496006	4.278122
1	0.612928	-0.372327	4.361638
1	-0.318971	0.652992	6.408134
6	-0.556437	1.070591	5.435241
6	-1.392774	2.178991	5.331935
1	-1.817426	2.628719	6.223881
1	-2.394567	3.538018	3.986110
6	-1.716106	2.695748	4.081755
6	-1.930939	1.743951	0.638191
6	-2.673020	0.600354	0.962573
1	-2.955014	0.427215	1.995890
6	-3.030451	-0.308212	-0.027810
1	-3.602808	-1.189676	0.243516
1	-2.951669	-0.799342	-2.124855
6	-2.669784	-0.089748	-1.354626
6	-1.943202	1.054162	-1.681161
1	-1.649444	1.236315	-2.710074
1	-0.987328	2.841831	-0.954153
6	-1.570343	1.962795	-0.698862
5	0.459506	0.443104	1.755757
1	0.265293	4.321255	2.644162
6	1.292474	1.398867	0.820344
1	2.336379	1.327237	1.161522
1	1.289682	1.065216	-0.222272
1	1.007172	2.453415	0.865475
6	0.482349	-1.105809	1.488615
1	0.204306	-1.728948	2.342682
1	-0.280549	-1.271541	0.711744
1	1.427805	-1.457754	1.064955

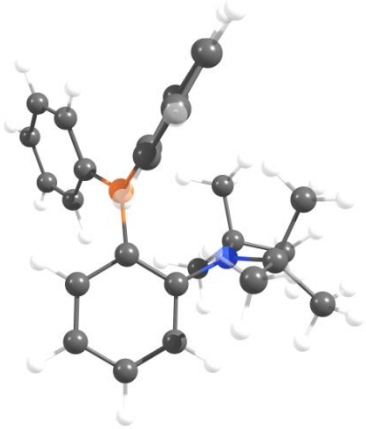

Figure S28: Computed structure of Ph/t-but (FLP)

Data for system: **Ph/t-but (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1089.57152538 A.U.
Zero-point correction= 0.524222 (Hartree/Particle)
Thermal correction to Energy= 0.550548
Thermal correction to Enthalpy= 0.551492
Thermal correction to Gibbs Free Energy= 0.470057

Optimized Geometry (XYZ coordinates in Å)

6	-1.359647	3.976977	1.247987
6	0.003543	4.348381	1.192424
5	1.225187	3.365092	1.043524
7	-1.776909	2.624296	1.051439
6	0.326805	5.711840	1.328330
1	1.369760	6.011649	1.252475
6	-0.638055	6.682063	1.573172
1	-0.350798	7.720990	1.698807
6	-2.325465	4.973132	1.444767
1	-3.372103	4.682677	1.442120
6	-1.976295	6.305650	1.630505
1	-2.749945	7.049948	1.792904
6	1.473506	2.222414	2.091089
6	1.319140	2.492583	3.458654
6	1.901667	0.933415	1.730296
6	1.555507	1.518488	4.425621
6	2.114156	-0.053908	2.686951
6	1.938779	0.237396	4.039103
1	1.012028	3.489300	3.767840
1	2.053380	0.698010	0.679638
1	1.430916	1.756202	5.477487
1	2.421209	-1.049125	2.380705
1	2.107388	-0.530412	4.787744
6	2.307542	3.649812	-0.059472
6	3.596802	3.092331	0.015704
6	2.029169	4.482494	-1.159601
6	4.556703	3.344680	-0.959067
6	2.977534	4.728943	-2.145681
6	4.244896	4.158241	-2.045596
1	3.852394	2.461835	0.862249
1	1.050575	4.948895	-1.235481
1	5.547156	2.909065	-0.872737
1	2.733589	5.367876	-2.988533
1	4.990223	4.352489	-2.810983
6	-2.430736	1.916797	2.191108
6	-1.785919	2.115626	-0.354472
6	-3.974054	1.806288	2.109369
1	-4.321469	1.012930	1.448849
1	-4.367514	1.587724	3.107389
1	-4.416102	2.750219	1.777430
6	-1.826675	0.512022	2.359813
1	-1.975963	-0.117157	1.480091
1	-0.752713	0.583312	2.557589
1	-2.304877	0.007638	3.206037
6	-2.142431	2.669648	3.502643
1	-2.437480	2.027479	4.337057
1	-1.082606	2.896417	3.604576
1	-2.707062	3.601282	3.578254
6	-1.805267	3.289810	-1.349679

1	-0.915415	3.915692	-1.268272
1	-1.841493	2.889042	-2.366558
1	-2.683404	3.922896	-1.192830
6	-0.540336	1.264291	-0.656164
1	-0.411076	0.466196	0.077275
1	-0.613909	0.816612	-1.653445
1	0.363371	1.882858	-0.652155
6	-3.033284	1.281686	-0.695744
1	-2.976453	1.001234	-1.751299
1	-3.104866	0.357525	-0.121404
1	-3.947118	1.862330	-0.550903

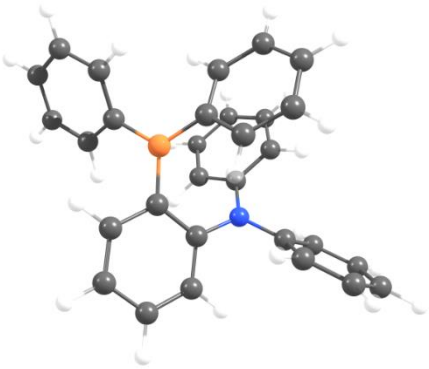

Figure S29: Computed structure of Ph/Ph (FLP)

Data for system: **Ph/Ph (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1237.22773399 A.U.
Zero-point correction= 0.459440 (Hartree/Particle)
Thermal correction to Energy= 0.484724
Thermal correction to Enthalpy= 0.485668
Thermal correction to Gibbs Free Energy= 0.402755

Optimized Geometry (XYZ coordinates in Å)

6	-1.350551	4.385926	1.530525
6	0.000026	4.657040	1.209602
5	1.071745	3.588770	0.764684
7	-1.901694	3.084681	1.377641
6	0.440239	5.983348	1.353208
1	1.469043	6.214739	1.089686
6	-0.379060	6.997183	1.838657
1	0.005629	8.004496	1.956971
6	-2.188749	5.412418	1.980948
1	-3.228361	5.187880	2.195722
6	-1.701727	6.702161	2.152522
1	-2.368335	7.480657	2.510392
6	1.196173	2.223318	1.517108
6	0.718888	2.081739	2.830197
6	1.697786	1.075975	0.880340
6	0.732756	0.854450	3.481862
6	1.709970	-0.159556	1.521487

6	1.226349	-0.271478	2.822547
1	0.328593	2.957657	3.341887
1	2.041241	1.147680	-0.148287
1	0.352524	0.770728	4.495338
1	2.086137	-1.036679	1.003874
1	1.231670	-1.234892	3.323577
6	2.080156	3.971914	-0.374427
6	3.397372	3.482682	-0.386609
6	1.703920	4.839851	-1.414819
6	4.296254	3.839724	-1.387683
6	2.586806	5.182110	-2.432577
6	3.888262	4.683068	-2.417651
1	3.723761	2.821960	0.411868
1	0.697486	5.251484	-1.419769
1	5.312628	3.459088	-1.366721
1	2.267239	5.843423	-3.231937
1	4.584240	4.956254	-3.204998
6	-2.842783	2.609896	2.325419
6	-3.980502	1.908511	1.909217
6	-2.652624	2.842602	3.692852
6	-4.893078	1.434204	2.844200
6	-3.580124	2.380205	4.618875
6	-4.701863	1.667106	4.203696
1	-4.137630	1.733707	0.850044
1	-1.783551	3.402499	4.021444
1	-5.767953	0.890032	2.502780
1	-3.416894	2.572150	5.674663
1	-5.419488	1.300965	4.929890
6	-1.592169	2.293888	0.246540
6	-1.512701	0.900022	0.360985
6	-1.322408	2.891125	-0.989762
6	-1.164762	0.129113	-0.738772
6	-0.943990	2.109848	-2.078481
6	-0.867352	0.725875	-1.963829
1	-1.681661	0.435948	1.327618
1	-1.401679	3.968602	-1.089846
1	-1.092226	-0.948211	-0.626216
1	-0.717831	2.594087	-3.023291
1	-0.576723	0.119491	-2.814789

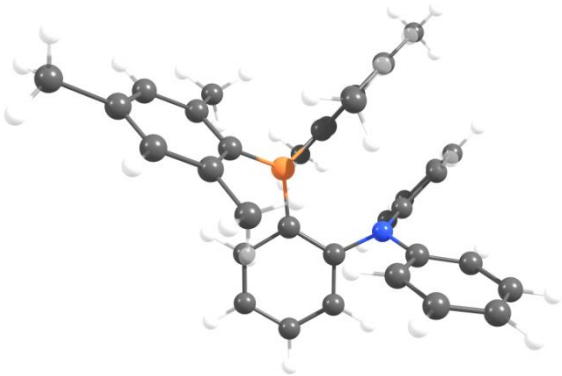

Figure S29: Computed structure of Ph/Mes (FLP)

Data for system: **Ph/Mes (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1473.07601559 A.U.
Zero-point correction= 0.626215 (Hartree/Particle)
Thermal correction to Energy= 0.661405
Thermal correction to Enthalpy= 0.662350
Thermal correction to Gibbs Free Energy= 0.559103

Optimized Geometry (XYZ coordinates in Å)

6	-1.209076	4.321818	1.404843
6	-0.071453	5.128500	1.606858
5	1.432467	4.689666	1.404357
7	-1.100693	2.952327	0.977355
6	-0.293570	6.447239	2.050760
1	0.571176	7.078082	2.242574
6	-1.567746	6.955876	2.268050
1	-1.697288	7.980490	2.601058
6	-2.490467	4.819012	1.662139
1	-3.339767	4.155008	1.526736
6	-2.674345	6.130042	2.082364
1	-3.676732	6.503539	2.266393
6	1.891019	3.769983	0.210140
6	1.779299	4.176879	-1.135679
6	1.201978	5.513804	-1.541226
1	1.995379	6.199284	-1.859134
1	0.645023	5.995002	-0.733205
1	0.520268	5.387625	-2.386698
6	2.253287	3.349980	-2.153535
1	2.153868	3.679167	-3.187030
6	2.823335	2.108755	-1.886467
1	2.464185	1.010153	-3.699762
6	3.290756	1.226458	-3.014146
1	4.078388	1.711916	-3.598424
1	3.681881	0.276751	-2.642133
1	3.318448	0.718662	-0.326736
6	2.903766	1.698140	-0.557674
6	2.450614	2.505023	0.485027
6	2.480084	1.968596	1.896049
1	2.995853	1.006641	1.942674
1	2.983065	2.658069	2.581375
1	1.456899	1.813239	2.264378
6	2.501241	5.268633	2.425705
6	3.633274	5.980875	1.968195
6	3.870363	6.250097	0.500398
1	3.011694	6.754360	0.046936
1	4.038127	5.325321	-0.057974
1	4.740517	6.896485	0.365855
6	4.552221	6.501852	2.880544
1	5.405402	7.062790	2.504824
6	4.411462	6.320423	4.252520
1	6.167995	6.069809	5.473192
6	5.439167	6.846861	5.219824
1	5.988940	7.689497	4.794155
1	4.973207	7.175709	6.152225
1	3.167103	5.457453	5.772233
6	3.299209	5.613106	4.703339
6	2.346039	5.103625	3.823642

6	1.179836	4.344320	4.413037
1	1.324157	4.189189	5.484729
1	0.236887	4.882066	4.271682
1	1.071208	3.359840	3.948378
6	-1.687430	1.981176	1.831732
6	-1.530568	2.115487	3.218925
6	-2.439155	0.903054	1.346202
6	-2.084134	1.185423	4.088777
6	-2.980581	-0.027768	2.227488
6	-2.807016	0.099292	3.601762
1	-0.983975	2.966438	3.607607
1	-2.602746	0.792822	0.280979
1	-1.944096	1.313186	5.157666
1	-3.557678	-0.855467	1.826833
1	-3.233476	-0.629901	4.281817
6	-1.035566	2.702463	-0.420443
6	-0.452286	1.512041	-0.874688
6	-1.529523	3.616183	-1.353589
6	-0.387698	1.236666	-2.231616
6	-1.439688	3.340141	-2.717283
6	-0.876366	2.151550	-3.165444
1	-0.042065	0.816830	-0.148960
1	-1.973112	4.546632	-1.015223
1	0.073090	0.310932	-2.563595
1	-1.824757	4.063592	-3.429855
1	-0.813978	1.938326	-4.227490

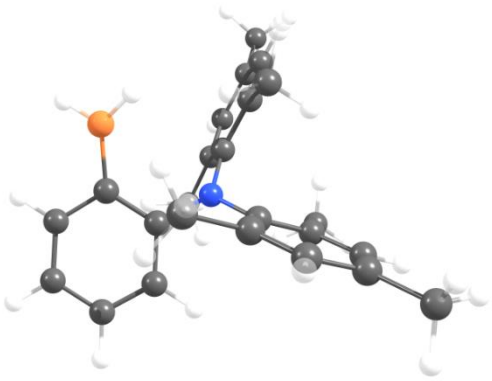

Figure S30: Computed structure of Mes/H (FLP)

Data for system: **Mes/H (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1010.96486169 A.U.
Zero-point correction= 0.460448 (Hartree/Particle)
Thermal correction to Energy= 0.486154
Thermal correction to Enthalpy= 0.487098
Thermal correction to Gibbs Free Energy= 0.405802

Optimized Geometry (XYZ coordinates in Å)

6	-0.041523	3.370428	0.148095

6	1.354894	3.601635	0.130879
5	2.407663	2.490709	-0.056242
7	-0.566580	2.149169	-0.312744
6	1.812110	4.885189	0.481011
1	2.880777	5.078720	0.433998
6	0.952314	5.881800	0.924201
1	1.332617	6.855972	1.210989
6	-0.912482	4.370665	0.598139
1	-1.980924	4.178086	0.613173
6	-0.413140	5.605419	0.993333
1	-1.105022	6.371152	1.331580
6	-1.753527	1.630912	0.291418
6	-2.877443	1.306934	-0.488761
6	-1.769408	1.407401	1.685206
6	-3.988733	0.741132	0.140552
6	-2.911849	0.862792	2.264475
1	-4.853286	0.485667	-0.468296
1	-2.915585	0.684238	3.337907
6	-4.033151	0.514739	1.512104
6	-0.009183	1.499066	-1.458982
6	0.225830	0.109612	-1.426002
6	0.246595	2.229908	-2.638991
6	0.711925	-0.517461	-2.571344
6	0.762301	1.554274	-3.745598
1	0.890285	-1.590142	-2.537335
1	0.956225	2.122852	-4.652746
6	0.999841	0.183239	-3.740294
6	-0.047572	3.703128	-2.774836
1	-0.163146	3.960929	-3.829797
1	-0.960559	3.988405	-2.246984
1	0.756944	4.318796	-2.358872
6	0.000562	-0.711447	-0.183805
1	-1.061773	-0.903612	-0.000953
1	0.512210	-1.671934	-0.274158
1	0.390856	-0.195205	0.697667
6	1.571661	-0.515423	-4.946512
1	2.663955	-0.567084	-4.888057
1	1.198164	-1.539444	-5.024984
1	1.315838	0.013209	-5.868041
6	-2.931011	1.555060	-1.974454
1	-2.526607	2.538381	-2.226184
1	-2.348894	0.816461	-2.535470
1	-3.965418	1.511182	-2.321816
6	-5.256772	-0.065615	2.172782
1	-5.909862	-0.548296	1.442329
1	-4.983139	-0.807150	2.928253
1	-5.838264	0.713910	2.675857
6	-0.580947	1.716927	2.558777
1	-0.630508	1.133967	3.480908
1	0.360890	1.492507	2.050679
1	-0.546497	2.778321	2.827367
1	3.525948	2.791675	-0.348616
1	2.162448	1.351823	0.196995

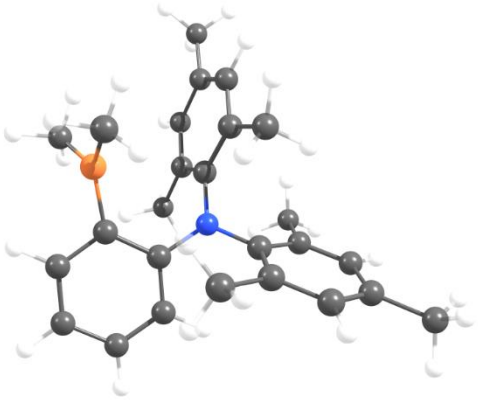

Figure S31: Computed structure of Mes/CH3 (FLP)

Data for system: **Mes/CH3 (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1089.61559146 A.U.
Zero-point correction= 0.517552 (Hartree/Particle)
Thermal correction to Energy= 0.546581
Thermal correction to Enthalpy= 0.547525
Thermal correction to Gibbs Free Energy= 0.459174

Optimized Geometry (XYZ coordinates in Å)

6	0.413137	2.755851	0.446567
6	1.789870	2.477149	0.327468
5	2.411912	1.341110	-0.573279
7	-0.523781	2.063931	-0.359289
6	2.676019	3.250547	1.089185
6	2.237740	4.218923	1.988134
1	2.950716	4.783781	2.579123
6	-0.033729	3.751284	1.323615
1	-1.096274	3.967060	1.383706
6	0.872306	4.461354	2.102392
1	0.506358	5.224951	2.781810
6	-1.869922	1.898062	0.087541
6	-2.121167	1.296814	1.340913
6	-2.946654	2.287814	-0.730689
6	-3.439759	1.101003	1.741559
6	-4.249759	2.045398	-0.289681
1	-3.623882	0.629292	2.704871
1	-5.076041	2.342736	-0.931774
6	-4.523364	1.460977	0.941780
6	-0.145673	1.627106	-1.662428
6	-0.456042	0.315034	-2.083684
6	0.494469	2.517494	-2.554352
6	-0.077021	-0.087166	-3.362070
6	0.872816	2.050880	-3.814585
1	-0.312904	-1.102042	-3.675680
1	1.373116	2.740832	-4.491138
6	0.607399	0.753732	-4.239561
6	0.749822	3.966631	-2.224506

1	0.773216	4.553788	-3.145410
1	-0.019236	4.377034	-1.566836
1	1.704133	4.104788	-1.705115
6	-1.177825	-0.667336	-1.197997
1	-2.256227	-0.474615	-1.177261
1	-1.017293	-1.684925	-1.560978
1	-0.827182	-0.608226	-0.165882
6	1.051917	0.267007	-5.594309
1	2.013118	-0.253465	-5.527056
1	0.329118	-0.433110	-6.020801
1	1.175467	1.098585	-6.292106
6	-1.012418	0.835880	2.250802
1	-0.154218	0.464232	1.685882
1	-0.639188	1.655089	2.874396
1	-1.372299	0.041347	2.908194
6	-5.938198	1.242123	1.411523
1	-6.049614	0.263908	1.887192
1	-6.228985	1.998333	2.148087
1	-6.644517	1.299124	0.580253
6	-2.751666	2.964350	-2.063723
1	-3.687073	3.427375	-2.384919
1	-1.987616	3.742749	-2.005513
1	-2.434439	2.261004	-2.841023
6	3.550651	1.698394	-1.608487
1	4.517453	1.502392	-1.121213
1	3.516012	1.045880	-2.486644
1	3.560380	2.740381	-1.938685
6	2.148457	-0.182513	-0.263573
1	1.270840	-0.386051	0.352485
1	2.091692	-0.784755	-1.176166
1	3.024642	-0.545073	0.294039
1	3.744815	3.073326	0.985649

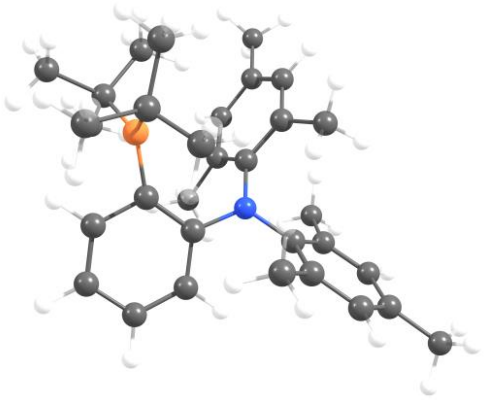

Figure S32: Computed structure of Mes/t-but (FLP

Data for system: **Mes/t-but (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1325.42559001 A.U.
Zero-point correction= 0.691633 (Hartree/Particle)
Thermal correction to Energy= 0.727697

Thermal correction to Enthalpy= 0.728641
Thermal correction to Gibbs Free Energy= 0.626941

Optimized Geometry (XYZ coordinates in Å)

6	0.510098	2.566251	0.452072
6	1.905212	2.320614	0.352434
5	2.833754	1.199494	-0.314592
7	-0.451805	1.839784	-0.311141
6	2.745559	3.165605	1.103397
1	3.823943	3.019497	1.030417
6	2.280841	4.165731	1.950191
1	2.977818	4.773633	2.516725
6	0.044964	3.598884	1.280375
1	-1.022568	3.791422	1.318900
6	0.910159	4.375936	2.036725
1	0.509096	5.160705	2.670216
6	-1.840979	1.798456	0.073965
6	-2.190695	1.322028	1.363891
6	-2.882586	2.170962	-0.811149
6	-3.527595	1.285970	1.750281
6	-4.209320	2.070384	-0.374439
1	-3.763790	0.926445	2.749407
1	-4.995212	2.355337	-1.069883
6	-4.564087	1.652706	0.898682
6	-0.116359	1.528832	-1.663124
6	-0.404610	0.251536	-2.172581
6	0.367801	2.545272	-2.521209
6	-0.134385	-0.012407	-3.519590
6	0.623272	2.227243	-3.851581
1	-0.356939	-1.004004	-3.908470
1	0.988726	3.010301	-4.513334
6	0.394666	0.950975	-4.371420
6	0.481577	3.985567	-2.077976
1	0.529715	4.636551	-2.954452
1	-0.378134	4.281577	-1.471212
1	1.362732	4.174242	-1.460614
6	-1.119896	-0.796030	-1.358626
1	-2.202165	-0.717079	-1.517980
1	-0.805662	-1.799039	-1.658056
1	-0.954263	-0.674830	-0.288822
6	0.738420	0.629379	-5.801556
1	1.803909	0.392033	-5.895653
1	0.172998	-0.232470	-6.163216
1	0.532064	1.477428	-6.459636
6	-1.188596	0.771583	2.342980
1	-0.734988	-0.141665	1.950895
1	-0.378881	1.467020	2.572025
1	-1.690534	0.516008	3.278249
6	-6.000583	1.606285	1.348335
1	-6.211868	0.687319	1.902015
1	-6.232235	2.446967	2.010474
1	-6.683161	1.655578	0.496938
6	-2.710277	2.680304	-2.226602
1	-3.679306	3.016822	-2.600209
1	-2.027927	3.526955	-2.287633
1	-2.337520	1.911552	-2.909987
6	3.859032	1.574417	-1.508433
6	2.955206	-0.197774	0.482347
6	3.773729	3.026988	-2.005552

1	3.869445	3.759977	-1.198965
1	4.582090	3.214110	-2.723278
1	2.834491	3.210289	-2.526670
6	5.335194	1.334561	-1.127980
1	5.538513	0.305855	-0.825531
1	5.968914	1.551025	-1.997052
1	5.660618	1.996682	-0.316683
6	3.520140	0.659263	-2.714436
1	3.915945	1.109474	-3.633738
1	3.965400	-0.331481	-2.614960
1	2.442458	0.530535	-2.853254
6	1.649768	-0.537793	1.200654
1	0.830350	-0.651592	0.487634
1	1.747080	-1.476367	1.761545
1	1.382700	0.252312	1.903888
6	3.356048	-1.430877	-0.342951
1	4.347005	-1.346153	-0.793600
1	3.371867	-2.312780	0.309597
1	2.634716	-1.625661	-1.144210
6	4.009266	0.021887	1.597917
1	4.068008	-0.889295	2.206584
1	5.010969	0.228294	1.215709
1	3.719841	0.841523	2.263663

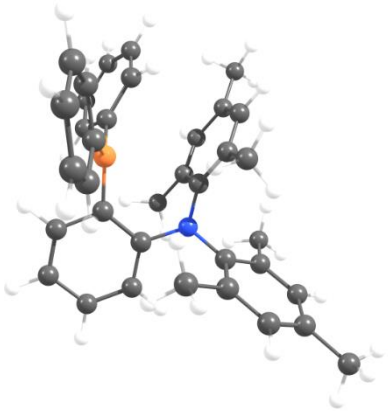

Figure S33: Computed structure of Mes/Ph (FLP)

Data for system: **Mes/Ph (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1473.08259096 A.U.
Zero-point correction= 0.627626 (Hartree/Particle)
Thermal correction to Energy= 0.662393
Thermal correction to Enthalpy= 0.663337
Thermal correction to Gibbs Free Energy= 0.561645

Optimized Geometry (XYZ coordinates in Å)

6	0.423522	3.084650	0.130350
6	1.773261	2.672224	0.145586
5	2.355338	1.213188	-0.080783
7	-0.617216	2.182389	-0.201690

6	2.739038	3.639227	0.471949
1	3.785215	3.338784	0.511425
6	2.411445	4.955899	0.778590
1	3.188790	5.669651	1.029444
6	0.090956	4.410138	0.444793
1	-0.954711	4.703249	0.421904
6	1.071998	5.334810	0.773012
1	0.788087	6.354887	1.012011
6	-1.916780	2.321317	0.381412
6	-2.046874	2.333652	1.788897
6	-3.076234	2.401470	-0.418781
6	-3.312834	2.447581	2.358142
6	-4.322444	2.484022	0.206785
1	-3.393541	2.452052	3.443193
1	-5.208885	2.539557	-0.421380
6	-4.470433	2.520705	1.588426
6	-0.424497	1.255948	-1.269087
6	-0.710113	-0.104204	-1.057574
6	-0.013666	1.707987	-2.543642
6	-0.628988	-0.984188	-2.140152
6	0.079477	0.785783	-3.579085
1	-0.857264	-2.035105	-1.975022
1	0.407434	1.132067	-4.557170
6	-0.237080	-0.562261	-3.405984
6	0.310043	3.151890	-2.825847
1	0.257323	3.343655	-3.899844
1	-0.370584	3.834583	-2.311948
1	1.318538	3.405128	-2.483377
6	-1.074366	-0.630319	0.305962
1	-2.052192	-0.271160	0.642364
1	-1.094331	-1.722153	0.295932
1	-0.336117	-0.311617	1.049331
6	-0.135358	-1.521754	-4.561978
1	-0.210722	-2.558693	-4.225885
1	-0.932022	-1.346802	-5.292320
1	0.819912	-1.397391	-5.081417
6	-0.860367	2.177383	2.698146
1	-0.253657	3.088542	2.746016
1	-1.188774	1.930069	3.709942
1	-0.208015	1.377904	2.341190
6	-5.826729	2.656950	2.230024
1	-5.879337	2.094879	3.166101
1	-6.047598	3.703857	2.463529
1	-6.616057	2.292495	1.568369
6	-3.051654	2.417815	-1.927113
1	-4.029605	2.724002	-2.304609
1	-2.308713	3.120097	-2.308855
1	-2.814916	1.436313	-2.349261
6	2.817303	0.750071	-1.508069
6	2.679145	-0.572607	-1.960090
6	3.396452	1.675982	-2.392775
6	3.097331	-0.954285	-3.231441
6	3.826170	1.300866	-3.661282
6	3.674216	-0.018168	-4.085355
1	2.196631	-1.307131	-1.321565
1	3.514207	2.709748	-2.075588
1	2.964431	-1.981613	-3.558355
1	4.276572	2.036042	-4.321109
1	4.004260	-0.313959	-5.076707
6	2.687998	0.363946	1.199028

6	2.352272	0.852351	2.475988
6	3.389479	-0.855860	1.148433
6	2.645674	0.142170	3.634938
6	3.688538	-1.573392	2.301244
6	3.306029	-1.080788	3.547138
1	1.869365	1.820941	2.554742
1	3.729778	-1.237850	0.192345
1	2.368488	0.544711	4.604164
1	4.230067	-2.511478	2.230876
1	3.539363	-1.640018	4.448216

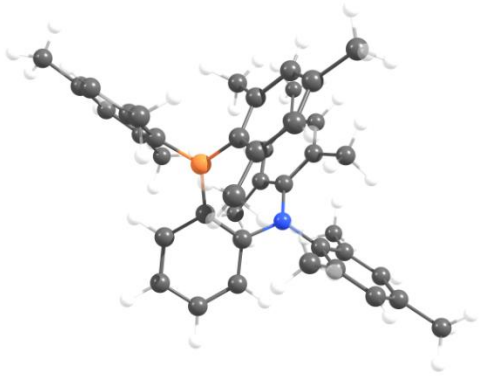

Figure S34: Computed structure of Mes/Mes (FLP)

Data for system: **Mes/Mes (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1708.93424125 A.U.
Zero-point correction= 0.795986 (Hartree/Particle)
Thermal correction to Energy= 0.839062
Thermal correction to Enthalpy= 0.840006
Thermal correction to Gibbs Free Energy= 0.721844

Optimized Geometry (XYZ coordinates in Å)

6	-0.367882	3.447753	0.633618
6	0.969132	3.545634	1.131173
5	1.938731	2.472379	1.775017
7	-1.005140	2.222028	0.307007
6	1.489143	4.853194	1.274178
1	2.517359	4.950868	1.612897
6	0.753056	6.007879	1.048327
1	1.199238	6.984363	1.201747
6	-1.100326	4.621955	0.393277
1	-2.107992	4.531662	0.000776
6	-0.562454	5.880179	0.615454
1	-1.166702	6.759916	0.415416
6	-2.441899	2.127293	0.339678
6	-3.204752	1.701716	-0.770642
6	-3.106491	2.421052	1.552313
6	-4.593084	1.595582	-0.627234
6	-4.491438	2.323534	1.628301
1	-5.169254	1.264356	-1.488100

1	-4.975174	2.556493	2.574786
6	-5.263687	1.907173	0.547589
6	-0.291688	1.202928	-0.392704
6	-0.456609	-0.137433	0.003030
6	0.442635	1.520494	-1.554330
6	0.157030	-1.136509	-0.752290
6	1.064243	0.484105	-2.252856
1	0.032349	-2.171822	-0.440487
1	1.635215	0.729030	-3.146316
6	0.939625	-0.850093	-1.868971
6	1.428682	1.232059	2.619299
6	0.674718	1.354799	3.804497
6	1.845108	-0.063030	2.225145
6	0.288787	0.209287	4.510745
6	1.440101	-1.179520	2.949929
1	-0.298677	0.327196	5.419855
1	1.751721	-2.167644	2.614785
6	0.644289	-1.066659	4.091390
6	3.526007	2.697799	1.734156
6	4.298654	2.674475	2.922549
6	4.230642	2.862511	0.517535
6	5.689261	2.776338	2.870170
6	5.623550	2.937436	0.500314
1	6.250177	2.768213	3.802436
1	6.130982	3.043630	-0.456485
6	6.378259	2.887794	1.667058
6	3.675550	2.606365	4.296664
1	3.225882	1.630340	4.498218
1	4.429107	2.799947	5.063476
1	2.893806	3.362033	4.406390
6	7.882927	2.938203	1.628135
1	8.288624	3.371753	2.545426
1	8.302878	1.932038	1.525049
1	8.237666	3.530743	0.781143
6	0.481969	2.916285	-2.128944
1	0.901892	2.891300	-3.137189
1	-0.519560	3.352002	-2.181157
1	1.074468	3.607715	-1.527821
6	-1.304969	-0.514492	1.187540
1	-2.372064	-0.465115	0.943893
1	-1.069647	-1.531197	1.509571
1	-1.123176	0.161010	2.028140
6	1.652046	-1.945051	-2.618726
1	2.633207	-2.143959	-2.173331
1	1.083836	-2.878163	-2.593356
1	1.814918	-1.670467	-3.663806
6	-2.645678	1.337035	-2.126210
1	-1.977628	2.103249	-2.518334
1	-2.085729	0.397102	-2.105843
1	-3.468954	1.224408	-2.834580
6	-6.760510	1.782661	0.662220
1	-7.212783	1.546675	-0.303577
1	-7.036389	0.990005	1.364906
1	-7.207186	2.711756	1.028074
6	2.754430	-0.265730	1.035276
1	3.784841	0.008547	1.284404
1	2.741815	-1.310695	0.714683
1	2.446612	0.340712	0.177466
6	0.351687	2.688587	4.443971
1	1.040059	2.877084	5.274164

1	0.428256	3.524208	3.743507
1	-0.656865	2.688396	4.864700
6	0.173752	-2.294236	4.826620
1	-0.688656	-2.741931	4.320514
1	0.958024	-3.054662	4.870649
1	-0.129882	-2.054181	5.848205
6	-2.339371	2.791375	2.785642
1	-2.939646	2.603177	3.679293
1	-1.428594	2.195168	2.839531
1	-2.036704	3.844363	2.789855
6	3.525216	2.971673	-0.809127
1	4.223799	2.811114	-1.634201
1	2.719503	2.243112	-0.906896
1	3.088240	3.968394	-0.929960

3.2 Dimers

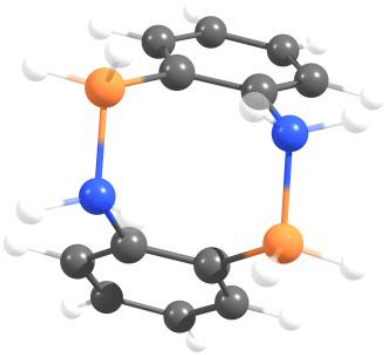

Figure S35: Computed structure of H/H

Data for system: **H/H**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -626.13497659 A.U.
Zero-point correction= 0.269902 (Hartree/Particle)
Thermal correction to Energy= 0.282688
Thermal correction to Enthalpy= 0.283632
Thermal correction to Gibbs Free Energy= 0.231126

Optimized Geometry (XYZ coordinates in Å)

6	2.416689	4.664761	2.281061
6	1.092378	5.081255	2.115991
5	-0.017745	4.904600	3.268036
7	2.746374	4.003578	3.539122
6	0.798083	5.672711	0.882367
1	-0.218059	6.013443	0.704840
6	1.759999	5.833351	-0.113208
1	1.492571	6.298573	-1.056686
6	3.397393	4.791897	1.308186

1	4.404603	4.425078	1.489311
6	3.061757	5.388501	0.096206
1	3.814163	5.501132	-0.677325
1	3.723082	4.164433	3.778740
1	0.321997	5.367376	4.344363
1	-1.099857	5.306171	2.918559
1	2.186587	4.452783	4.267996
6	-0.512574	1.132805	0.569821
6	0.791234	0.653957	0.485932
1	1.070274	-0.016510	-0.320721
1	-1.255043	0.842746	-0.166220
6	-0.863295	1.993103	1.606307
6	1.740225	1.042254	1.429867
1	2.758189	0.671576	1.349243
6	1.430430	1.902207	2.489395
6	0.104683	2.343414	2.536251
1	-1.872404	2.389818	1.684617
7	-0.240637	3.276472	3.603467
5	2.525587	2.340914	3.584240
1	3.611816	1.872069	3.350363
1	2.171677	2.137600	4.733710
1	0.308975	3.008178	4.423485
1	-1.220512	3.173020	3.861192

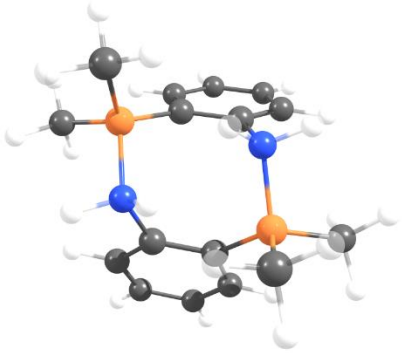

Figure S36: Computed structure of H/CH3

Data for system: **H/CH3**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -783.40407236 A.U.
Zero-point correction= 0.383372 (Hartree/Particle)
Thermal correction to Energy= 0.402670
Thermal correction to Enthalpy= 0.403614
Thermal correction to Gibbs Free Energy= 0.338625

Optimized Geometry (XYZ coordinates in Å)

6	2.371446	4.655488	1.749933
6	1.057978	5.061601	1.486206
5	-0.196772	4.865531	2.508180
7	2.635361	3.917336	2.982165
6	0.884197	5.729756	0.265922
1	-0.110746	6.070326	-0.003078

6	1.932927	5.976468	-0.617141
1	1.744016	6.500414	-1.548769
6	3.440493	4.878371	0.890320
1	4.435461	4.531371	1.156985
6	3.218996	5.549053	-0.307303
1	4.044704	5.733805	-0.986259
1	3.578978	4.125852	3.310566
1	2.009299	4.276822	3.703490
6	-0.671882	0.859046	0.162679
6	0.626421	0.378690	0.034700
1	0.861956	-0.353360	-0.731318
1	-1.460884	0.509721	-0.494846
6	-0.953507	1.797636	1.149057
6	1.627600	0.838734	0.886989
1	2.633524	0.450423	0.762092
6	1.392369	1.780663	1.898469
6	0.069135	2.229308	1.985278
1	-1.959293	2.191558	1.270237
7	-0.255677	3.242197	2.986002
5	2.590838	2.226874	2.909264
1	0.329225	3.072950	3.804950
1	-1.216536	3.112627	3.304916
6	-1.630402	5.133322	1.806414
1	-1.769835	4.590312	0.863732
1	-2.467631	4.868952	2.468652
1	-1.757188	6.198387	1.581287
6	-0.065879	5.700119	3.902484
1	-0.912297	5.501287	4.573825
1	0.842379	5.550505	4.507290
1	-0.093444	6.771732	3.678787
6	4.058691	1.805721	2.372600
1	4.860639	2.227283	2.995983
1	4.189622	0.718614	2.418895
1	4.253323	2.105554	1.335701
6	2.378384	1.753777	4.454915
1	1.439420	2.039330	4.954947
1	2.410811	0.660104	4.499389
1	3.188119	2.115086	5.103315

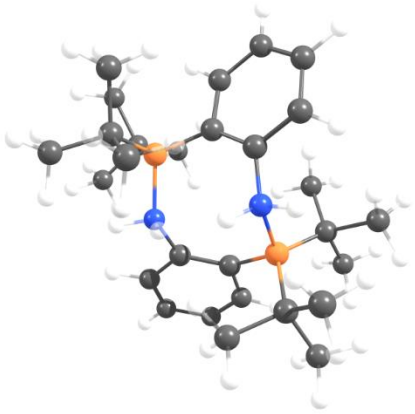

Figure S37: Computed structure of H/t-but

Data for system: **H/t-but**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1255.01724994 A.U.
Zero-point correction= 0.729441 (Hartree/Particle)
Thermal correction to Energy= 0.763079
Thermal correction to Enthalpy= 0.764023
Thermal correction to Gibbs Free Energy= 0.671424

Optimized Geometry (XYZ coordinates in Å)

6	2.778647	4.738732	1.980245
6	1.579202	5.240135	1.450021
5	0.008988	4.869691	1.783161
7	2.841914	3.514985	2.800868
6	1.753861	6.438194	0.720702
1	0.884848	6.907636	0.289236
6	2.962248	7.101681	0.557663
1	2.998370	8.020688	-0.018480
6	3.991982	5.430327	1.894404
1	4.864394	5.044737	2.413639
6	4.102877	6.607135	1.174613
1	5.053611	7.125193	1.113664
1	3.775781	3.509187	3.215282
1	2.237080	3.650083	3.607868
6	-1.266915	0.128604	1.373709
6	-0.080106	-0.413760	0.896553
1	-0.078662	-1.362149	0.369202
1	-2.214346	-0.384827	1.252345
6	-1.213440	1.361664	2.001561
6	1.119606	0.241608	1.141816
1	2.023802	-0.250117	0.814348
6	1.237339	1.475728	1.813360
6	-0.000118	2.041063	2.145615
1	-2.131745	1.814465	2.364732
7	-0.129483	3.406226	2.665998
5	2.733327	1.869581	2.362994
1	0.395547	3.504307	3.536041
1	-1.097580	3.489154	2.974589
6	-0.496399	5.940460	3.014909
6	-0.943383	4.686952	0.415083
6	3.969640	1.599825	1.260007
6	2.875482	1.157084	3.897498
6	-1.688821	5.443043	3.870953
1	-2.542132	5.110594	3.271816
1	-1.415611	4.633883	4.562450
1	-2.049847	6.256964	4.510769
6	-0.928020	7.316765	2.482182
1	-0.161521	7.785217	1.859849
1	-1.853271	7.251979	1.901967
1	-1.119904	7.998124	3.321983
6	0.647158	6.202148	4.017766
1	1.049779	5.273608	4.457733
1	1.484196	6.734825	3.558249
1	0.288072	6.801617	4.864116
6	-1.012347	5.906121	-0.541047
1	-0.101260	6.006037	-1.135677
1	-1.827302	5.738043	-1.256603
1	-1.212992	6.858641	-0.045663
6	-0.415772	3.553303	-0.499422

1	0.666149	3.644087	-0.650482
1	-0.616417	2.548786	-0.128374
1	-0.894577	3.627227	-1.484811
6	-2.419869	4.397349	0.755131
1	-2.961125	4.095213	-0.150544
1	-2.564881	3.591953	1.480616
1	-2.920421	5.289392	1.147683
6	4.508887	0.150682	1.194481
1	5.051807	-0.119405	2.105829
1	3.759040	-0.623883	1.029261
1	5.223982	0.076662	0.364960
6	5.240603	2.446001	1.521104
1	5.550443	2.479831	2.572346
1	6.085635	2.021934	0.965744
1	5.123065	3.465184	1.154499
6	3.508239	2.004441	-0.156295
1	4.348521	1.952721	-0.861715
1	2.711547	1.363784	-0.542339
1	3.130810	3.034157	-0.166179
6	2.606963	-0.359675	3.849503
1	2.778594	-0.799260	4.840949
1	1.571776	-0.574167	3.569489
1	3.257483	-0.881189	3.145351
6	4.258938	1.345256	4.550187
1	4.268568	0.896566	5.552096
1	5.055260	0.869700	3.972851
1	4.538407	2.399531	4.691792
6	1.840365	1.700252	4.910228
1	0.814027	1.590970	4.539917
1	1.895383	1.130248	5.845774
1	2.005664	2.746968	5.211021

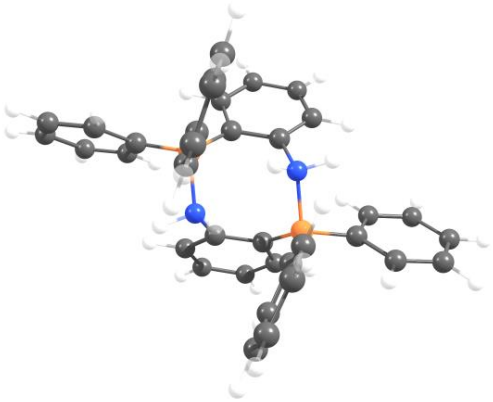

Figure S38: Computed structure of H/Ph

Data for system: **H/Ph**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1550.35303321 A.U.
Zero-point correction= 0.601317 (Hartree/Particle)
Thermal correction to Energy= 0.633129
Thermal correction to Enthalpy= 0.634073

Thermal correction to Gibbs Free Energy= 0.537435

Optimized Geometry (XYZ coordinates in Å)

6	2.326826	4.638180	0.726272
6	0.960788	4.867108	0.501878
5	-0.177410	4.520792	1.614703
7	2.729238	3.970776	1.962728
6	0.661978	5.570085	-0.673487
1	-0.374130	5.814821	-0.882795
6	1.642722	5.986463	-1.572319
1	1.357967	6.527757	-2.468918
6	3.328316	5.052691	-0.143872
1	4.370182	4.855327	0.093124
6	2.981718	5.723320	-1.312394
1	3.755931	6.050261	-1.998433
1	3.666860	4.286999	2.213468
1	2.112962	4.311669	2.710211
6	-0.133822	0.329737	-0.698018
6	1.216477	0.015438	-0.786046
1	1.555205	-0.739964	-1.487878
1	-0.862881	-0.169820	-1.327202
6	-0.551827	1.280916	0.227168
6	2.138370	0.657918	0.038802
1	3.183304	0.373246	-0.026587
6	1.768291	1.642329	0.965501
6	0.392985	1.914136	1.025930
1	-1.604780	1.527931	0.331019
7	-0.083205	2.880195	2.013942
5	2.832508	2.277635	2.022086
1	0.485727	2.755274	2.859076
1	-1.035506	2.631150	2.284855
6	0.131034	5.311455	3.008592
6	0.623340	6.628167	2.961900
6	-0.086597	4.772248	4.287053
6	0.884746	7.360073	4.116257
6	0.180966	5.491253	5.452295
6	0.669183	6.790351	5.370108
1	0.806837	7.084213	1.991491
1	-0.477460	3.761494	4.405278
1	1.262713	8.375183	4.038970
1	0.008720	5.030391	6.420375
1	0.879876	7.355171	6.272760
6	-1.706231	4.712405	1.109020
6	-2.147059	4.183008	-0.118190
6	-2.674464	5.338568	1.906230
6	-3.476820	4.264379	-0.522601
6	-4.008715	5.430743	1.510080
6	-4.415635	4.890774	0.294809
1	-1.426851	3.703183	-0.777914
1	-2.378235	5.769023	2.859408
1	-3.779822	3.845843	-1.478003
1	-4.729896	5.927298	2.152591
1	-5.453214	4.960835	-0.017048
6	2.424412	1.898103	3.556117
6	1.803996	0.669637	3.843362
6	2.674894	2.741175	4.651906
6	1.446462	0.308479	5.140100
6	2.317566	2.394780	5.954043
6	1.697357	1.174577	6.202285

1	1.593279	-0.015524	3.025153
1	3.165562	3.703381	4.505732
1	0.967980	-0.649281	5.321892
1	2.521039	3.081660	6.770121
1	1.413698	0.899307	7.213212
6	4.388902	1.972492	1.685523
6	5.297318	1.570538	2.674502
6	4.912012	2.175486	0.394754
6	6.652464	1.386253	2.399846
6	6.263234	2.000038	0.109272
6	7.141404	1.604245	1.116327
1	4.937106	1.392562	3.684437
1	4.239814	2.468581	-0.409239
1	7.325752	1.069779	3.191053
1	6.630364	2.164533	-0.899655
1	8.195540	1.461954	0.898954

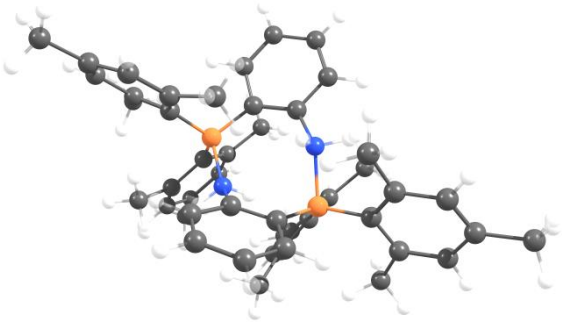

Figure S39: Computed structure of H/Mes

Data for system: **H/Mes**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -2021.99445979 A.U.
Zero-point correction= 0.936845 (Hartree/Particle)
Thermal correction to Energy= 0.987307
Thermal correction to Enthalpy= 0.988251
Thermal correction to Gibbs Free Energy= 0.855557

Optimized Geometry (XYZ coordinates in Å)

6	1.750383	6.712878	3.304481
6	0.394449	6.889706	2.998687
5	-0.758504	5.904309	2.390065
7	2.440659	5.402070	3.393194
6	-0.105225	8.183573	3.263683
1	-1.165590	8.353597	3.094267
6	0.666704	9.242545	3.710350
1	0.213954	10.214122	3.880107
6	2.546919	7.775619	3.758421
1	3.596387	7.595553	3.985496
6	2.025741	9.044773	3.938779
1	2.663020	9.851597	4.284268
1	3.398614	5.636086	3.650664

1	2.061387	4.977046	4.239358
6	-0.318671	1.291424	4.261990
6	1.027896	0.938731	4.319624
1	1.330096	0.031963	4.833906
1	-1.072507	0.670065	4.734016
6	-0.696225	2.442466	3.580961
6	1.988390	1.751198	3.722867
1	3.036981	1.470068	3.784880
6	1.654540	2.932809	3.043750
6	0.288201	3.229676	2.989602
1	-1.738961	2.743145	3.516431
7	-0.140900	4.343976	2.152290
5	2.777830	3.948257	2.421600
1	-0.840158	3.946863	1.530611
1	0.631981	4.560239	1.512246
1	-2.786940	7.826413	1.524791
1	-4.445350	7.951548	2.127436
6	-3.631268	7.254401	1.911684
1	-3.964254	6.603927	1.097498
6	-3.291648	6.485181	3.175139
6	-2.015439	5.929970	3.458342
6	-4.334308	6.392290	4.103182
1	-5.301229	6.819645	3.843048
6	-4.179290	5.787190	5.344015
6	-2.901072	5.355084	5.676486
1	-2.717767	4.957444	6.673270
6	-1.830873	5.457004	4.784552
6	-0.469580	5.176781	5.387108
1	-0.033515	6.114566	5.752786
1	0.229111	4.738503	4.681905
1	-0.551981	4.486247	6.230784
1	-5.843194	4.675907	6.147832
6	-5.335641	5.634966	6.297150
1	-4.999996	5.669945	7.336827
1	-6.076722	6.424638	6.149622
1	-3.866394	4.154417	0.498209
6	-2.842467	4.173744	0.880648
1	-2.905162	4.326862	1.957137
1	-2.438529	3.167006	0.693254
6	-2.042454	5.246940	0.144282
6	-2.310647	5.291639	-1.223073
1	-3.035137	4.591861	-1.638418
6	-1.689821	6.205437	-2.064789
6	-1.997543	6.250224	-3.539019
1	-1.839518	5.272763	-4.006349
1	-3.040950	6.529005	-3.716946
1	-1.363370	6.977617	-4.052140
6	-0.779782	7.070923	-1.479383
1	-0.272877	7.796073	-2.113112
1	0.109718	8.914004	0.849744
6	0.560653	8.092001	0.287693
1	1.368394	7.685385	0.895130
1	1.011268	8.514811	-0.614093
6	-0.467754	7.050229	-0.112365
6	-1.109027	6.133458	0.763634
1	0.337607	2.188710	0.575400
6	1.355042	2.210758	0.167092
1	1.983016	1.658307	0.866827
1	1.328978	1.657594	-0.775048
6	1.867195	3.616257	-0.097918

6	1.619329	4.109435	-1.379279
1	1.029818	3.506335	-2.067802
6	2.114491	5.336023	-1.811674
6	1.844084	5.836756	-3.205720
1	2.534986	5.385188	-3.925786
1	0.825666	5.588404	-3.516651
1	1.963387	6.921956	-3.264300
6	2.925975	6.035627	-0.929511
1	3.384413	6.968681	-1.254845
1	3.729934	7.326897	1.541911
6	4.179206	6.407710	1.153923
1	4.634871	5.852113	1.975897
1	4.995356	6.708641	0.490819
6	3.181213	5.580833	0.367718
6	2.599927	4.384494	0.851021
6	5.023698	2.783201	0.548510
1	4.094670	2.228328	0.411624
1	5.837876	2.170769	0.153398
1	4.951103	3.683654	-0.067208
6	5.293498	3.094348	2.007689
6	6.605710	2.864022	2.424577
6	7.016196	3.038821	3.741376
6	8.449988	2.827221	4.150485
1	7.332667	2.524194	1.689381
1	8.885962	1.968306	3.633481
1	9.060021	3.702050	3.902357
1	8.534616	2.658419	5.226640
6	6.039720	3.394977	4.658711
1	6.308930	3.476848	5.710277
1	4.192752	3.443865	6.359550
6	3.792148	3.927535	5.466118
1	2.781623	3.535807	5.330736
1	3.724652	4.996761	5.706069
6	4.711593	3.632122	4.284792
6	4.303209	3.550525	2.922785

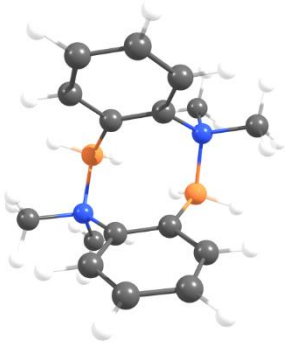

Figure S40: Computed structure of CH3/H

Data for system: **CH3/H**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -783.30835283 A.U.

Zero-point correction= 0.385647 (Hartree/Particle)
Thermal correction to Energy= 0.402783
Thermal correction to Enthalpy= 0.403727
Thermal correction to Gibbs Free Energy= 0.343066

Optimized Geometry (XYZ coordinates in Å)

6	2.734058	4.333703	2.110464
6	1.529864	5.005876	1.816316
5	0.446838	4.670911	0.662620
7	3.227056	3.264615	1.193498
6	1.188222	6.055418	2.682536
1	0.284856	6.616270	2.457050
6	1.938634	6.411796	3.798855
1	1.621390	7.229651	4.438140
6	3.492901	4.671251	3.231827
1	4.402352	4.144588	3.483395
6	3.093430	5.701280	4.080011
1	3.699703	5.941165	4.947475
1	-0.233767	5.647887	0.453661
1	0.843553	4.211320	-0.367608
6	-0.348888	1.648643	4.545850
6	0.790837	0.892401	4.330135
1	1.147210	0.198919	5.085304
1	-0.903646	1.570179	5.475203
6	-0.800431	2.514037	3.552302
6	1.474923	1.040401	3.127397
1	2.366370	0.443116	2.954104
6	1.079705	1.921218	2.109236
6	-0.108563	2.641969	2.347213
1	-1.696319	3.082265	3.757834
7	-0.659365	3.532012	1.283522
5	2.092819	2.037789	0.853638
1	1.634802	2.305818	-0.217921
1	2.765911	1.035942	0.785425
6	3.643134	3.895857	-0.093244
1	4.470758	4.586355	0.094541
1	3.955745	3.101107	-0.772739
1	2.796266	4.426330	-0.518102
6	4.428870	2.576244	1.731850
1	4.171707	2.085278	2.671238
1	4.729840	1.823774	1.007244
1	5.246181	3.285802	1.882370
6	-1.147350	2.681931	0.158091
1	-0.323989	2.080059	-0.214728
1	-1.957775	2.040006	0.516086
1	-1.505199	3.343271	-0.632908
6	-1.831034	4.312630	1.758921
1	-2.176816	4.925691	0.930447
1	-2.635191	3.646201	2.080393
1	-1.522208	4.961220	2.579586

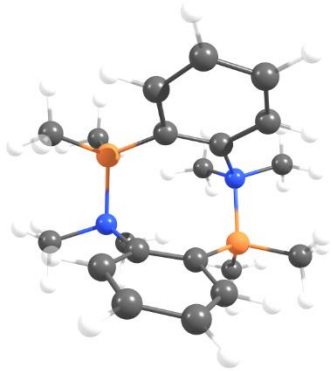

Figure S41: Computed structure of CH3/H

Data for system: **CH3/H**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -940.51363232 A.U.
Zero-point correction= 0.501418 (Hartree/Particle)
Thermal correction to Energy= 0.524797
Thermal correction to Enthalpy= 0.525741
Thermal correction to Gibbs Free Energy= 0.452145

Optimized Geometry (XYZ coordinates in Å)

6	3.028388	4.272398	1.876264
6	1.962751	5.202834	1.684787
5	0.533255	5.249025	0.765157
7	3.161763	2.995289	1.110307
6	2.101893	6.348956	2.499667
1	1.362558	7.129256	2.423926
6	3.106751	6.579336	3.431025
1	3.109248	7.501794	4.002913
6	4.015977	4.469112	2.846945
1	4.775633	3.721968	3.015904
6	4.068815	5.610248	3.631655
1	4.854393	5.724405	4.371102
6	-0.811432	3.462974	4.828383
6	0.162735	2.541914	5.156321
1	0.295047	2.202436	6.178699
1	-1.472556	3.891022	5.574460
6	-0.937318	3.830729	3.498028
6	1.005481	2.068097	4.158586
1	1.767380	1.383109	4.492492
6	0.960107	2.415391	2.789559
6	-0.115290	3.307151	2.494748
1	-1.704177	4.550945	3.258890
7	-0.429750	3.800472	1.118765
5	2.239938	1.713334	1.916937
6	2.800976	3.231633	-0.308861
1	3.497023	3.956729	-0.740949
1	2.857459	2.287804	-0.852153
1	1.815517	3.642571	-0.376172
6	4.588517	2.557815	0.988188

1	5.024197	2.270412	1.933818
1	4.602447	1.685979	0.332725
1	5.170017	3.369337	0.543673
6	-0.276444	2.687511	0.149752
1	0.705306	2.267916	0.219494
1	-0.995482	1.899153	0.391426
1	-0.458283	3.065030	-0.857089
6	-1.879528	4.138743	0.958409
1	-2.037613	4.384886	-0.092452
1	-2.478326	3.266606	1.232416
1	-2.181857	4.990829	1.549169
6	1.929927	0.511128	0.842265
1	1.398952	0.682996	-0.097346
1	2.866246	0.008249	0.567444
1	1.341406	-0.240808	1.382836
6	3.299088	1.007087	2.947092
1	3.722860	1.650488	3.728635
1	2.796921	0.176980	3.454113
1	4.126850	0.531677	2.414299
6	0.617149	5.460440	-0.861069
1	1.240570	6.348578	-1.023932
1	1.010126	4.695416	-1.535274
1	-0.374194	5.722452	-1.252976
6	-0.397313	6.509528	1.241550
1	0.131157	7.441535	1.017039
1	-1.318028	6.578034	0.656170
1	-0.667205	6.542320	2.304842

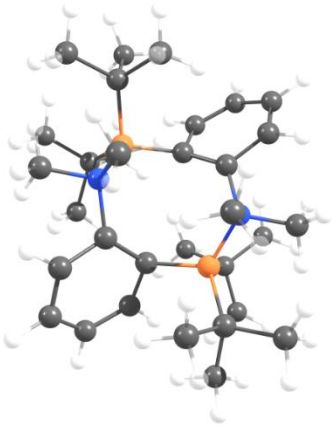

Figure S42: Computed structure of CH3/t-but

Data for system: **CH3/t-but**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1412.01799724 A.U.
Zero-point correction= 0.849809 (Hartree/Particle)
Thermal correction to Energy= 0.886161
Thermal correction to Enthalpy= 0.887105
Thermal correction to Gibbs Free Energy= 0.791885

Optimized Geometry (XYZ coordinates in Å)

6	0.217869	1.896586	-0.444762
6	1.168202	1.099143	0.269499
5	1.989465	-0.400496	0.085146
7	-1.200963	1.531697	-0.876559
6	-1.273338	-1.110624	0.129945
6	-0.330757	-1.858210	-0.629286
7	1.081512	-1.435970	-1.043002
5	-2.041571	0.389948	0.138460
6	3.497914	0.126733	-0.754074
6	2.298274	-1.340584	1.506627
6	-2.131185	1.051571	1.745930
6	-3.600782	-0.010700	-0.731999
6	4.385739	-0.903541	-1.519543
1	4.746726	-1.725616	-0.895584
1	3.924727	-1.334765	-2.412793
1	5.275910	-0.378084	-1.883882
6	4.510854	0.737636	0.267020
1	4.272803	1.770877	0.514427
1	4.607807	0.181084	1.196969
1	5.505766	0.762444	-0.192798
6	3.330612	1.275132	-1.788899
1	2.921439	0.949284	-2.748653
1	2.722627	2.102038	-1.421848
1	4.322814	1.687980	-2.014094
6	2.542056	-0.519201	2.805017
1	1.712099	0.145631	3.051638
1	2.641839	-1.222593	3.640056
1	3.464593	0.067032	2.794876
6	1.152886	-2.286771	1.954373
1	0.263496	-1.736301	2.249371
1	0.836438	-3.027334	1.219620
1	1.494920	-2.850080	2.831838
6	3.553192	-2.256713	1.430824
1	3.709175	-2.711089	2.417309
1	3.457202	-3.089431	0.732011
1	4.471737	-1.723568	1.184860
6	-3.515458	0.932018	2.416462
1	-4.277131	1.510191	1.881695
1	-3.876507	-0.094428	2.509259
1	-3.456191	1.339514	3.434189
6	-1.787391	2.552382	1.965770
1	-2.546520	3.229174	1.567081
1	-1.766760	2.736165	3.045656
1	-0.802233	2.841964	1.588699
6	-1.138109	0.342609	2.695087
1	-1.113032	0.858937	3.662956
1	-1.398964	-0.695118	2.904878
1	-0.130553	0.357967	2.279362
6	-4.713184	-0.674910	0.139652
1	-5.498794	-1.028866	-0.539421
1	-4.396141	-1.549111	0.703289
1	-5.192508	0.025071	0.821489
6	-4.439503	1.126862	-1.387954
1	-5.334031	0.679348	-1.837248
1	-4.801725	1.852562	-0.650039
1	-3.952827	1.686596	-2.189865
6	-3.406295	-1.075657	-1.853350
1	-3.075126	-2.034937	-1.450959
1	-4.374298	-1.254949	-2.338495

1	-2.717063	-0.803025	-2.651917
6	-1.222818	1.090816	-2.300987
1	-0.985475	0.040816	-2.359537
1	-2.217982	1.231292	-2.707312
1	-0.509863	1.690036	-2.875539
6	-2.048908	2.791487	-0.854548
1	-3.030052	2.537564	-0.486437
1	-1.623797	3.535633	-0.201734
1	-2.129819	3.206119	-1.861320
6	1.129109	-0.827148	-2.404869
1	2.111503	-1.002912	-2.831752
1	0.377996	-1.302535	-3.042612
1	0.981765	0.242531	-2.344392
6	1.909111	-2.684870	-1.192486
1	1.688375	-3.392070	-0.403494
1	1.724188	-3.148581	-2.163431
1	2.945913	-2.407902	-1.139615
6	1.984944	1.932202	1.075863
1	2.639963	1.444715	1.774197
6	2.118078	3.310301	0.994509
1	2.791007	3.830664	1.668488
6	0.518776	3.240360	-0.732792
1	-0.062209	3.763339	-1.482355
6	1.472651	3.966151	-0.041477
1	1.651671	5.009542	-0.275753
6	-2.098806	-1.959250	0.910137
1	-2.722310	-1.475217	1.646627
6	-2.237888	-3.328897	0.779770
1	-2.907392	-3.878405	1.433606
6	-0.622942	-3.200066	-0.945040
1	-0.049524	-3.717076	-1.700344
6	-1.578611	-3.943503	-0.275081
1	-1.746369	-4.982034	-0.538315

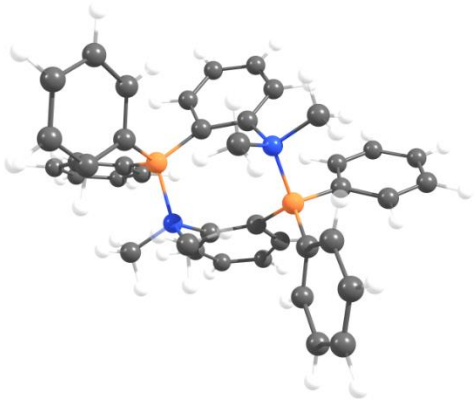

Figure S43: Computed structure of CH3/Ph

Data for system: **CH3/Ph**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1707.44998948 A.U.
Zero-point correction= 0.717147 (Hartree/Particle)

Thermal correction to Energy= 0.753227
Thermal correction to Enthalpy= 0.754171
Thermal correction to Gibbs Free Energy= 0.651625

Optimized Geometry (XYZ coordinates in Å)

6	2.565234	4.556897	1.229309
6	1.273333	5.045378	0.894081
5	-0.250689	4.998464	1.595043
7	2.852180	3.763157	2.472826
6	1.281115	5.921452	-0.218217
1	0.354290	6.409531	-0.484711
6	2.385043	6.234446	-0.997710
1	2.280194	6.921548	-1.831028
6	3.677641	4.835049	0.422159
1	4.640146	4.402914	0.643279
6	3.600377	5.649541	-0.695906
1	4.488452	5.831775	-1.291763
6	-0.828272	0.806306	-0.649708
6	0.409652	0.199990	-0.549295
1	0.675602	-0.647798	-1.172237
1	-1.571115	0.478304	-1.369102
6	-1.125675	1.840765	0.222666
6	1.326610	0.700310	0.363521
1	2.277451	0.188948	0.414830
6	1.114838	1.795558	1.235428
6	-0.207203	2.313598	1.170641
1	-2.102741	2.287149	0.132720
7	-0.736762	3.350654	2.121188
5	2.452053	2.028392	2.222433
6	4.310420	3.864526	2.835318
1	4.589708	4.919858	2.858751
1	4.440029	3.436437	3.824645
1	4.947912	3.318251	2.153214
6	2.214310	4.472282	3.626333
1	1.171995	4.662856	3.447999
1	2.334177	3.873519	4.528024
1	2.701406	5.442961	3.749768
6	-2.241020	3.297110	2.172413
1	-2.702126	3.666315	1.266231
1	-2.545343	2.266226	2.364574
1	-2.570557	3.928274	2.992112
6	-0.381684	2.921785	3.510515
1	-0.907837	1.989579	3.731556
1	0.669395	2.721186	3.607260
1	-0.678897	3.697526	4.214602
6	-0.349909	6.103236	2.815723
6	-1.278082	6.126892	3.871995
6	0.501930	7.224350	2.753472
6	-1.343479	7.163035	4.803691
6	0.442834	8.271384	3.668370
6	-0.479313	8.246182	4.709843
1	-2.002262	5.329558	3.995215
1	1.243078	7.283438	1.962757
1	-2.080366	7.118856	5.600231
1	1.125062	9.110176	3.565012
1	-0.526700	9.056877	5.429868
6	-1.392547	5.340284	0.464648
6	-1.395600	4.726894	-0.803854
6	-2.447218	6.227673	0.721994

6	-2.409593	4.942378	-1.731192
6	-3.466962	6.459487	-0.202814
6	-3.460527	5.807771	-1.430049
1	-0.571693	4.073128	-1.076863
1	-2.483260	6.752254	1.672112
1	-2.374140	4.442259	-2.694815
1	-4.265399	7.154468	0.040317
1	-4.253122	5.982071	-2.151262
6	3.803450	1.478149	1.467994
6	4.756553	0.694274	2.133784
6	4.096038	1.802855	0.128481
6	5.947424	0.294286	1.524860
6	5.282212	1.418132	-0.487628
6	6.222682	0.665317	0.214350
1	4.573471	0.388200	3.159448
1	3.366256	2.361274	-0.451454
1	6.658051	-0.311148	2.079892
1	5.468507	1.697356	-1.520704
1	7.148966	0.359658	-0.262433
6	2.257836	1.217472	3.645522
6	2.938834	1.444125	4.854849
6	1.407752	0.093306	3.648453
6	2.774431	0.639648	5.982433
6	1.240254	-0.725602	4.761199
6	1.919137	-0.453988	5.944840
1	3.642995	2.262624	4.952153
1	0.851050	-0.152500	2.749676
1	3.325664	0.871895	6.888864
1	0.572174	-1.579795	4.700188
1	1.788230	-1.085290	6.817894

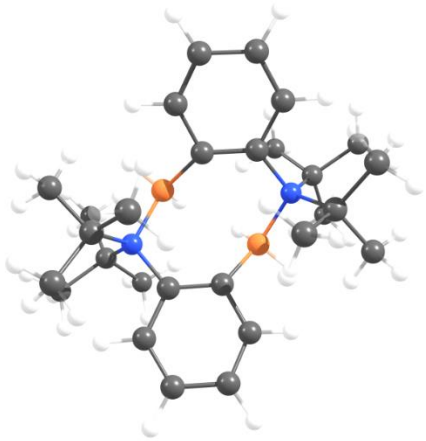

Figure S44: Computed structure of tbut/H

Data for system: **tbut/H**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1254.86453350 A.U.
Zero-point correction= 0.729863 (Hartree/Particle)
Thermal correction to Energy= 0.761606

Thermal correction to Enthalpy= 0.762550
Thermal correction to Gibbs Free Energy= 0.674293

Optimized Geometry (XYZ coordinates in Å)

6	2.738899	4.863988	2.190315
6	1.344906	4.987388	2.002329
5	0.200197	4.131520	1.167546
7	3.540276	3.616361	1.901434
6	0.830316	6.274884	2.321335
1	-0.233487	6.426892	2.181590
6	1.557503	7.359421	2.771695
1	1.064357	8.301911	2.987678
6	3.486927	5.984781	2.596396
1	4.552776	5.916315	2.670700
6	2.930644	7.213850	2.895050
1	3.569583	8.035726	3.201663
1	-0.596143	4.970734	0.889230
1	0.638693	3.695579	0.152421
6	-0.273284	-0.578341	3.218038
6	1.104605	-0.730476	3.202995
1	1.579581	-1.641396	3.553358
1	-0.933554	-1.364525	3.569758
6	-0.804970	0.608132	2.750162
6	1.863263	0.301162	2.685379
1	2.933500	0.139321	2.634090
6	1.374740	1.543491	2.193310
6	-0.028174	1.681027	2.274234
1	-1.873266	0.679747	2.746029
7	-0.804297	2.886503	1.798382
5	2.574334	2.307231	1.346121
1	2.203730	2.629363	0.263734
1	3.382888	1.444525	1.212240
6	4.479137	3.920152	0.619915
6	4.295564	3.171832	3.234925
6	-1.657965	2.440597	0.499092
6	-1.643775	3.472037	3.022657
6	4.888361	2.652700	-0.166481
1	5.390946	1.907663	0.447916
1	4.048123	2.184277	-0.669350
1	5.599404	2.984390	-0.928757
6	5.817314	4.626918	0.913461
1	5.730425	5.601823	1.385568
1	6.511679	4.001985	1.477021
1	6.278186	4.807956	-0.061081
6	3.688893	4.817089	-0.349636
1	4.208169	4.798074	-1.312158
1	2.671816	4.453069	-0.499690
1	3.642805	5.853290	-0.010448
6	3.226105	2.844103	4.291101
1	2.470228	3.632752	4.337195
1	2.732323	1.894011	4.123933
1	3.718492	2.797909	5.266462
6	5.211334	4.197361	3.958211
1	4.643436	4.966710	4.479841
1	5.737686	3.620475	4.723552
1	5.975551	4.662754	3.340916
6	5.194120	1.945762	3.004199
1	5.461442	1.552670	3.989260
1	4.711333	1.152048	2.444338

1	6.127400	2.214607	2.502948
6	-2.606326	2.527359	3.793285
1	-3.329414	1.993320	3.182112
1	-2.074833	1.822571	4.431478
1	-3.180165	3.181711	4.455143
6	-2.522793	4.660893	2.600538
1	-2.002164	5.391538	1.990763
1	-3.421594	4.334518	2.071309
1	-2.853501	5.157527	3.517238
6	-0.644473	3.920530	4.102890
1	-1.197603	4.065392	5.035070
1	0.109662	3.149001	4.279960
1	-0.144154	4.852332	3.866326
6	-3.014681	1.764411	0.779900
1	-3.410750	1.475200	-0.197032
1	-2.962156	0.847844	1.361418
1	-3.742932	2.444563	1.224155
6	-0.808573	1.446415	-0.312707
1	-0.788101	0.453760	0.140194
1	-1.263584	1.357967	-1.303468
1	0.217295	1.795961	-0.434588
6	-2.011269	3.612810	-0.445823
1	-2.672418	3.197059	-1.211760
1	-2.550311	4.418335	0.049781
1	-1.138872	4.026854	-0.941578

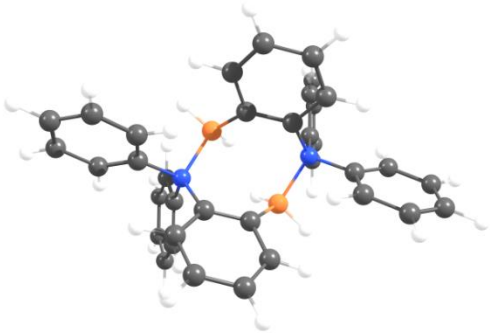

Figure S45: Computed structure of Ph/H

Data for system: **Ph/H**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1550.20761989 A.U.
Zero-point correction= 0.594776 (Hartree/Particle)
Thermal correction to Energy= 0.625482
Thermal correction to Enthalpy= 0.626426
Thermal correction to Gibbs Free Energy= 0.533835

Optimized Geometry (XYZ coordinates in Å)

6	2.916697	4.455753	2.188558
6	1.630198	4.998347	2.033738
5	0.539763	4.576075	0.923956
7	3.363092	3.317103	1.316047

6	1.378521	6.176431	2.761634
1	0.414674	6.655750	2.616556
6	2.298938	6.767399	3.618306
1	2.045035	7.675736	4.155737
6	3.870043	5.056354	3.016776
1	4.874293	4.659098	3.083270
6	3.557601	6.196853	3.747144
1	4.311835	6.644481	4.386134
1	-0.196413	5.504693	0.701494
1	1.029841	4.144543	-0.072510
6	-0.575955	1.055754	4.480171
6	0.672888	0.459052	4.376022
1	0.977194	-0.313932	5.074793
1	-1.271956	0.763957	5.259906
6	-0.956369	2.013952	3.547987
6	1.515706	0.842023	3.340047
1	2.468389	0.333345	3.223776
6	1.195852	1.837320	2.397569
6	-0.078532	2.412155	2.535011
1	-1.955157	2.425815	3.607764
7	-0.604668	3.339235	1.476269
5	2.189474	2.000630	1.138619
1	1.616892	2.210322	0.115160
1	2.913549	1.039374	1.063436
6	4.560224	2.655706	1.907338
6	4.445400	2.159028	3.208731
6	5.767767	2.535316	1.231747
6	5.515715	1.514219	3.808001
6	6.841165	1.882037	1.844145
6	6.722855	1.363531	3.124041
1	3.520748	2.305866	3.753366
1	5.894627	2.939584	0.236732
1	5.407414	1.134494	4.818785
1	7.776557	1.791194	1.301783
1	7.560487	0.858145	3.592660
6	3.679541	3.835509	-0.045586
6	3.947888	5.182761	-0.265301
6	3.776304	2.925864	-1.099897
6	4.288565	5.619648	-1.545120
6	4.125077	3.371216	-2.368484
6	4.378279	4.721560	-2.600023
1	3.877968	5.901355	0.541126
1	3.586391	1.875590	-0.920610
1	4.481735	6.674939	-1.706946
1	4.194839	2.654661	-3.180212
1	4.642380	5.067230	-3.593950
6	-1.755087	4.123937	2.005903
6	-3.014473	4.107906	1.420524
6	-1.538589	4.888988	3.155389
6	-4.039291	4.889341	1.962058
6	-2.561287	5.659080	3.685908
6	-3.821119	5.670985	3.085697
1	-3.218925	3.499538	0.550069
1	-0.571410	4.854522	3.641602
1	-5.016316	4.870607	1.490437
1	-2.373759	6.247434	4.578254
1	-4.621517	6.274609	3.500016
6	-1.026124	2.541950	0.289097
6	-1.216015	3.203256	-0.925445
6	-1.299282	1.181426	0.387933

6	-1.661989	2.497449	-2.035553
6	-1.738135	0.481433	-0.735562
6	-1.920737	1.131247	-1.948782
1	-1.021758	4.265757	-0.993296
1	-1.158241	0.653404	1.322218
1	-1.803366	3.022312	-2.974574
1	-1.934271	-0.582174	-0.649555
1	-2.260873	0.581292	-2.819982

4. Cartesian coordinates of aminoalanes

4.1 Monomers

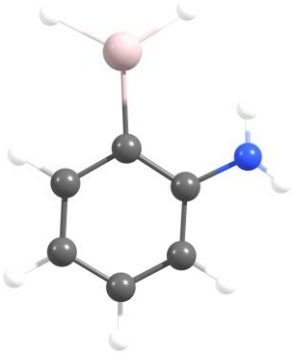

Figure S46: Computed structure of H/H (FLP)

Data for system: **H/H (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -530.595386506 A.U.
Zero-point correction= 0.121619 (Hartree/Particle)
Thermal correction to Energy= 0.129863
Thermal correction to Enthalpy= 0.130807
Thermal correction to Gibbs Free Energy= 0.089133

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.605321	4.815574	2.326664
6	1.245839	5.116045	2.063556
13	-0.186540	5.059213	3.360057
7	3.008477	4.358628	3.574064
6	0.908406	5.505254	0.753041
1	-0.131765	5.735296	0.526795
6	1.848723	5.609978	-0.264009
1	1.555589	5.915029	-1.262383
6	3.558284	4.920242	1.301407
1	4.597734	4.682984	1.512947
6	3.180134	5.313397	0.026616
1	3.935597	5.388026	-0.750137
1	3.988319	4.468598	3.787673

1	0.121556	4.810830	4.897890
1	-1.664290	5.311044	2.862291
1	2.404723	4.580691	4.352642

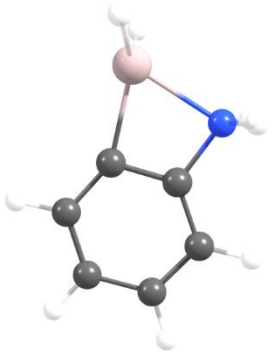

Figure S47: Computed structure of H/H (CLA)

Data for system: **H/H (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -530.614729754 A.U.
Zero-point correction= 0.123173 (Hartree/Particle)
Thermal correction to Energy= 0.130607
Thermal correction to Enthalpy= 0.131551
Thermal correction to Gibbs Free Energy= 0.091653

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.409165	4.833957	2.287812
6	1.087309	5.167768	1.988336
13	0.462089	4.793761	3.840327
7	2.529789	4.434656	3.701232
6	0.830944	5.567680	0.672985
1	-0.175009	5.842572	0.367681
6	1.860124	5.620034	-0.265111
1	1.648074	5.932347	-1.283265
6	3.463823	4.872243	1.382972
1	4.475430	4.600458	1.672500
6	3.168669	5.275259	0.084237
1	3.958045	5.321708	-0.658959
1	2.854019	3.475950	3.812470
1	0.266968	6.008276	4.845116
1	-0.230123	3.398583	4.151489
1	3.153856	5.042124	4.228618

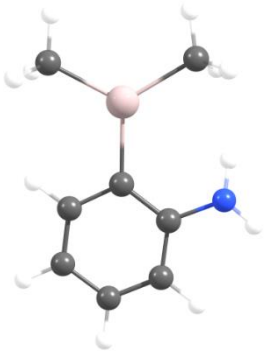

Figure S48: Computed structure of H/CH3 (FLP)

Data for system: **H/CH3 (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -609.248464981 A.U.
Zero-point correction= 0.180372 (Hartree/Particle)
Thermal correction to Energy= 0.192582
Thermal correction to Enthalpy= 0.193526
Thermal correction to Gibbs Free Energy= 0.141846

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.624473	4.692240	1.683870
6	1.325492	5.206034	1.455884
13	-0.216471	5.010313	2.632781
7	2.908199	3.955549	2.833530
6	1.110881	5.889133	0.245211
1	0.120478	6.294638	0.040722
6	2.106770	6.068280	-0.708925
1	1.902737	6.601645	-1.630964
6	3.632748	4.863842	0.724101
1	4.623509	4.456949	0.911255
6	3.372818	5.544200	-0.456826
1	4.169127	5.667275	-1.185087
1	3.890047	3.877146	3.056432
1	2.351203	4.183637	3.644415
6	-1.934924	5.674009	1.961977
1	-2.166410	5.268395	0.971246
1	-2.768389	5.425952	2.624701
1	-1.920652	6.764769	1.852689
6	-0.037183	4.215792	4.423064
1	-0.994221	4.156397	4.948634
1	0.372412	3.200242	4.370885
1	0.639568	4.796413	5.063245

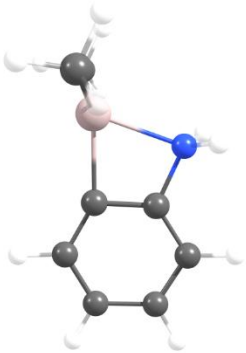

Figure S49: Computed structure of H/CH3 (CLA)

Data for system: **H/CH3 (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -609.263666614 A.U.
Zero-point correction= 0.181151 (Hartree/Particle)
Thermal correction to Energy= 0.192931
Thermal correction to Enthalpy= 0.193875
Thermal correction to Gibbs Free Energy= 0.143391

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.384759	4.780379	1.556342
6	1.166710	5.352217	1.182885
13	0.228544	4.709592	2.827181
7	2.257941	4.090993	2.851918
6	1.156790	6.039546	-0.036094
1	0.244860	6.511058	-0.393071
6	2.310762	6.132232	-0.812249
1	2.286598	6.669108	-1.755959
6	3.557743	4.849200	0.812745
1	4.478321	4.383456	1.154814
6	3.505682	5.541694	-0.393187
1	4.395954	5.622554	-1.008541
1	2.453108	3.093992	2.785424
1	2.867882	4.484293	3.565928
6	-0.869051	3.079647	2.706950
1	-0.488403	2.371854	1.962151
1	-0.928660	2.550673	3.664811
1	-1.899733	3.311972	2.416113
6	-0.010196	5.965716	4.324176
1	-0.066492	5.450420	5.289683
1	0.799770	6.700739	4.389015
1	-0.940126	6.536519	4.222623

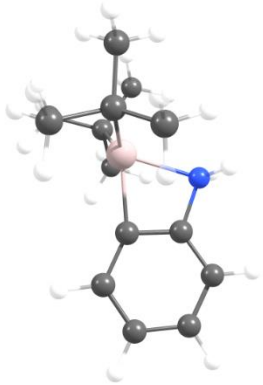

Figure S50: Computed structure of H/t-but (CLA)

Data for system: **H/t-but (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -845.095725289 A.U.
Zero-point correction= 0.352792 (Hartree/Particle)
Thermal correction to Energy= 0.372294
Thermal correction to Enthalpy= 0.373239
Thermal correction to Gibbs Free Energy= 0.305411

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.492541	5.537640	1.526600
6	1.418298	5.921236	2.332645
13	0.179817	4.600964	1.489188
7	2.090002	4.468674	0.594131
6	1.673336	6.939115	3.258293
1	0.884317	7.291069	3.917883
6	2.938297	7.517427	3.350983
1	3.121012	8.306239	4.074622
6	3.767966	6.087650	1.586892
1	4.567073	5.748713	0.932901
6	3.981198	7.095739	2.522476
1	4.960535	7.555587	2.606774
1	2.180937	4.751329	-0.380330
1	2.624882	3.611702	0.725926
6	-1.100700	5.341256	0.154508
6	-0.107830	2.864780	2.419909
6	-2.074544	6.254284	0.915919
1	-2.660185	5.699153	1.659928
1	-1.550411	7.062824	1.439997
1	-2.793165	6.724295	0.225928
6	-1.907331	4.268870	-0.585326
1	-1.263135	3.588542	-1.156519
1	-2.502262	3.656837	0.103052
1	-2.608932	4.727901	-1.300067
6	-0.346777	6.191655	-0.875880
1	0.283047	6.955171	-0.401623

1	0.294026	5.575625	-1.521530
1	-1.047856	6.716905	-1.543315
6	-0.149447	1.710286	1.410106
1	0.780188	1.635705	0.829449
1	-0.281659	0.744365	1.922965
1	-0.974866	1.815065	0.697252
6	1.033087	2.608924	3.412025
1	1.096621	3.392950	4.174494
1	0.894865	1.647741	3.931866
1	2.012350	2.562070	2.915540
6	-1.433970	2.891777	3.192217
1	-1.601742	1.940751	3.722330
1	-1.452352	3.687927	3.946921
1	-2.292218	3.045741	2.526622

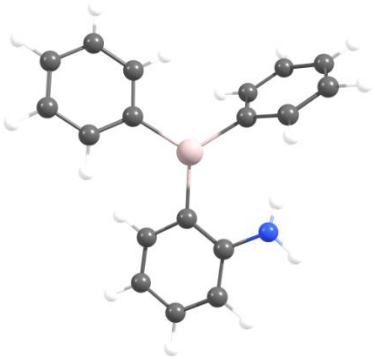

Figure S51: Computed structure of H/Ph (FLP)

Data for system: **H/Ph (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -992.711633146 A.U.
Zero-point correction= 0.291443 (Hartree/Particle)
Thermal correction to Energy= 0.309289
Thermal correction to Enthalpy= 0.310233
Thermal correction to Gibbs Free Energy= 0.243124

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.366766	4.189124	0.385905
6	1.161873	4.929194	0.416202
13	-0.340283	4.546529	1.594667
7	2.540021	3.098897	1.246853
6	1.043016	6.003729	-0.482542
1	0.137847	6.608512	-0.466103
6	2.038772	6.329524	-1.398939
1	1.911782	7.164299	-2.079546
6	3.366145	4.502694	-0.543683
1	4.281560	3.916466	-0.563664
6	3.197919	5.559252	-1.429350
1	3.986337	5.787538	-2.140411

1	3.491733	2.759623	1.289813
1	2.168799	3.241598	2.178994
6	-0.161652	3.671785	3.348456
6	-0.511849	4.388536	4.508062
6	0.248140	2.338067	3.527673
6	-0.445440	3.815326	5.776024
6	0.306809	1.751838	4.790638
6	-0.036994	2.491921	5.918414
1	-0.846030	5.422756	4.428794
1	0.535414	1.738953	2.664878
1	-0.714789	4.398680	6.651295
1	0.621659	0.717803	4.894360
1	0.011768	2.039379	6.903937
6	-2.130211	5.144598	1.096407
6	-2.476154	5.498122	-0.220641
6	-3.152672	5.190075	2.061340
6	-3.769176	5.891112	-0.555892
6	-4.446603	5.590572	1.737775
6	-4.754966	5.943959	0.426602
1	-1.724740	5.455078	-1.006208
1	-2.937884	4.896298	3.087299
1	-4.009416	6.153990	-1.581614
1	-5.215236	5.620949	2.504074
1	-5.763560	6.252821	0.169094

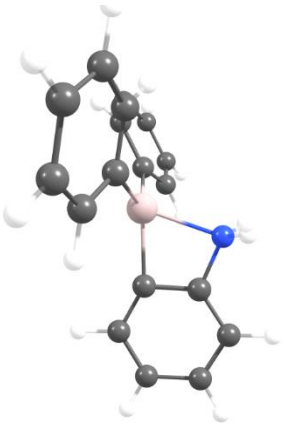

Figure S52: Computed structure of H/Ph (CLA)

Data for system: **H/Ph (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -992.732733632 A.U.
Zero-point correction= 0.291857 (Hartree/Particle)
Thermal correction to Energy= 0.309372
Thermal correction to Enthalpy= 0.310317
Thermal correction to Gibbs Free Energy= 0.243188

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.093851	4.291017	0.609362

6	1.014005	5.127829	0.318320
13	-0.142570	4.302731	1.708120
7	1.738912	3.350257	1.684804
6	1.213761	6.072204	-0.694292
1	0.417035	6.757001	-0.971908
6	2.435824	6.150377	-1.359513
1	2.578531	6.887356	-2.144103
6	3.328272	4.338222	-0.028873
1	4.135453	3.661681	0.238498
6	3.487723	5.291193	-1.030432
1	4.433297	5.366289	-1.557670
1	1.770558	2.376971	1.386943
1	2.322595	3.450051	2.513678
6	-0.264361	5.138407	3.482624
6	-1.417874	5.064914	4.280777
6	0.832317	5.835831	4.018612
6	-1.475041	5.646594	5.546366
6	0.790951	6.419211	5.282639
6	-0.367425	6.322635	6.050497
1	-2.297803	4.544825	3.905388
1	1.743826	5.942852	3.428285
1	-2.382456	5.574121	6.138838
1	1.655020	6.953090	5.667610
1	-0.407383	6.776984	7.035915
6	-1.515310	3.007464	1.166404
6	-1.875903	2.846001	-0.182540
6	-2.156493	2.171542	2.098367
6	-2.824845	1.907642	-0.583732
6	-3.104149	1.226725	1.710070
6	-3.440696	1.095348	0.364983
1	-1.404249	3.470070	-0.940388
1	-1.912636	2.258373	3.156672
1	-3.084894	1.809120	-1.633685
1	-3.581963	0.595417	2.453614
1	-4.181017	0.362823	0.057509

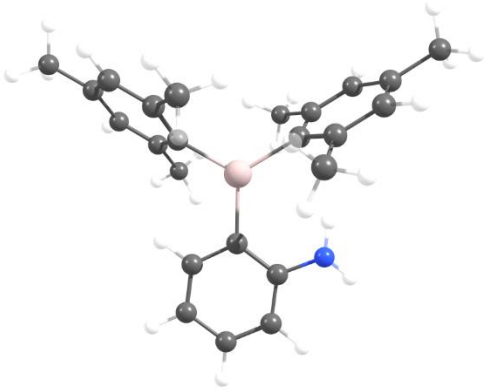

Figure S53: Computed structure of H/Mes (FLP)

Data for system: **H/Mes (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1228.58189509 A.U.
Zero-point correction= 0.457031 (Hartree/Particle)
Thermal correction to Energy= 0.485426
Thermal correction to Enthalpy= 0.486370
Thermal correction to Gibbs Free Energy= 0.395673

Optimized Geometry (XYZ coordinates in Angstrom)

6	1.900469	7.094762	3.602377
6	0.543278	7.274408	3.235590
13	-0.599642	5.959703	2.366337
7	2.578442	5.923020	3.294633
6	-0.044908	8.520030	3.530078
1	-1.089108	8.678422	3.259563
6	0.645475	9.550803	4.156123
1	0.158815	10.496469	4.367972
6	2.600783	8.133020	4.238560
1	3.641975	7.982686	4.512901
6	1.978086	9.341470	4.509688
1	2.540595	10.128333	5.003877
1	3.407530	5.734546	3.837392
1	2.018834	5.100664	3.110359
1	-1.176143	7.029641	-0.396615
1	-2.495401	6.406639	-1.384653
6	-1.998807	6.302213	-0.417216
1	-1.558785	5.298060	-0.374213
6	-2.954332	6.528708	0.733772
6	-2.484508	6.423728	2.061824
6	-4.282956	6.848040	0.475130
1	-4.625904	6.929637	-0.554900
6	-5.189053	7.072763	1.515654
6	-4.730609	6.965452	2.824049
1	-5.424015	7.135482	3.645724
6	-3.398661	6.643533	3.107390
6	-2.982716	6.491953	4.553544
1	-1.933353	6.766070	4.709347
1	-3.111164	5.456423	4.890565
1	-3.586668	7.122687	5.210996
1	-7.068197	6.723323	0.515585
6	-6.620314	7.435911	1.214288
1	-7.226390	7.448824	2.122765
1	-6.683491	8.426793	0.753392
1	-1.808511	2.206561	3.931937
6	-1.504656	3.175586	3.529420
1	-2.398291	3.670249	3.129884
1	-1.143069	3.777779	4.373893
6	-0.441043	3.033668	2.462851
6	0.019748	1.768668	2.109373
1	-0.388699	0.889932	2.605451
6	1.003358	1.603913	1.130720
6	1.476531	0.224885	0.749247
1	1.697026	-0.376214	1.635821
1	0.707967	-0.306386	0.178616
1	2.377906	0.270486	0.134179
6	1.520238	2.739945	0.514075
1	2.289357	2.627834	-0.247715
1	0.948639	5.571555	-0.645853
6	1.641198	5.219243	0.127567
1	1.838018	6.048825	0.816936
1	2.585012	4.977555	-0.367139

6	1.072470	4.020458	0.852317
6	0.082630	4.188103	1.840426

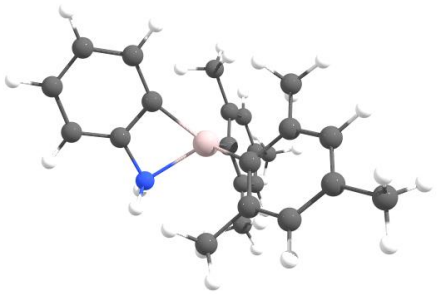

Figure S54: Computed structure of H/Mes (CLA)

Data for system: **H/Mes (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1228.59472826 A.U.
Zero-point correction= 0.458553 (Hartree/Particle)
Thermal correction to Energy= 0.486037
Thermal correction to Enthalpy= 0.486981
Thermal correction to Gibbs Free Energy= 0.398501

Optimized Geometry (XYZ coordinates in Angstrom)

6	1.676060	6.838710	3.767807
6	0.469083	7.519738	3.932253
13	-0.477229	6.393693	2.590939
7	1.526210	5.761534	2.773604
6	0.467900	8.566494	4.860245
1	-0.440705	9.135110	5.045110
6	1.626393	8.894728	5.561411
1	1.613528	9.711787	6.276551
6	2.852496	7.131073	4.449065
1	3.764812	6.564332	4.283411
6	2.812774	8.184051	5.357946
1	3.706361	8.452022	5.912331
1	2.180639	5.841721	1.998386
1	1.634816	4.836177	3.187906
1	1.894677	7.035423	0.160657
1	1.530231	6.388294	-1.436996
6	1.156569	6.459978	-0.412786
1	1.117503	5.444234	-0.003846
6	-0.198739	7.130720	-0.364109
6	-0.939733	7.185817	0.831850
6	-0.685933	7.713919	-1.536152
1	-0.096414	7.650387	-2.449190
6	-1.909290	8.378417	-1.565678
6	-2.644668	8.447776	-0.383602
1	-3.604139	8.962356	-0.383151
6	-2.176332	7.867994	0.794511
6	-3.012538	7.978926	2.051539

1	-2.451904	8.481034	2.851825
1	-3.311581	6.990396	2.422099
1	-3.922931	8.558520	1.882191
1	-1.943984	8.593034	-3.713570
6	-2.412829	9.029406	-2.828316
1	-3.496119	8.919156	-2.925320
1	-2.191453	10.101983	-2.830619
1	-2.999275	5.958548	6.148460
6	-2.273982	6.070917	5.338783
1	-2.533529	6.978522	4.782839
1	-1.290137	6.245504	5.785870
6	-2.263014	4.851826	4.442124
6	-2.985219	3.726213	4.844046
1	-3.543981	3.756826	5.777955
6	-3.009304	2.562085	4.078774
6	-3.822658	1.368250	4.508857
1	-3.904686	1.315851	5.597400
1	-4.839062	1.422121	4.104433
1	-3.377114	0.435772	4.153127
6	-2.283921	2.544090	2.889332
1	-2.288643	1.643648	2.277253
1	-1.044624	4.405768	0.496950
6	-0.791503	3.574238	1.164560
1	0.292813	3.609711	1.336510
1	-1.000594	2.641864	0.634798
6	-1.559226	3.659128	2.466613
6	-1.531034	4.843236	3.235105

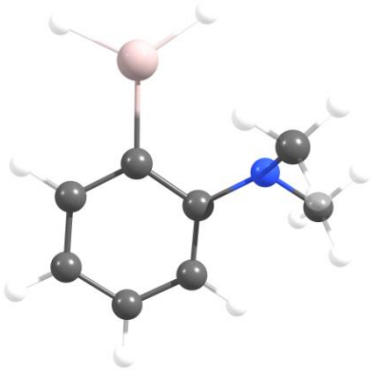

Figure S55: Computed structure of CH3/H (FLP)

Data for system: **CH3/H (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -609.188090802 A.U.
Zero-point correction= 0.178361 (Hartree/Particle)
Thermal correction to Energy= 0.189304
Thermal correction to Enthalpy= 0.190248
Thermal correction to Gibbs Free Energy= 0.141966

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.827491	4.541389	2.006278
6	1.520107	5.072312	1.906246
13	0.148104	4.376074	0.715460
7	3.230171	3.561827	1.056342
6	1.129656	6.037259	2.845389
1	0.124476	6.451998	2.791103
6	1.976655	6.461806	3.868744
1	1.645162	7.203407	4.587961
6	3.674481	4.953694	3.038455
1	4.675339	4.544957	3.124818
6	3.245383	5.905166	3.963319
1	3.918247	6.214451	4.757699
1	-1.275505	5.055549	0.874288
1	0.354294	3.225887	-0.347433
6	3.419142	4.067334	-0.298754
1	4.373325	4.610848	-0.403685
1	3.409474	3.232588	-1.005198
1	2.613022	4.750179	-0.569194
6	4.338065	2.708015	1.440418
1	4.169728	2.308964	2.442789
1	4.392642	1.871122	0.738851
1	5.313843	3.223683	1.423705

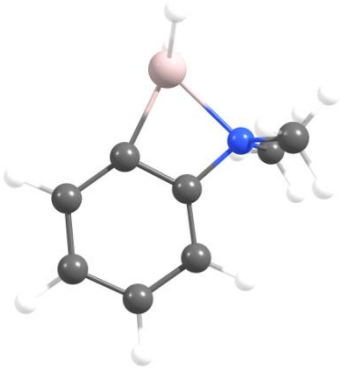

Figure S56: Computed structure of CH3/H (CLA)

Data for system: **CH3/H (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -609.217685146 A.U.
Zero-point correction= 0.179613 (Hartree/Particle)
Thermal correction to Energy= 0.189783
Thermal correction to Enthalpy= 0.190727
Thermal correction to Gibbs Free Energy= 0.144932

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.528905	4.594058	1.940484
6	1.229496	5.084489	2.072963
13	0.572889	3.983326	0.552112
7	2.612142	3.625010	0.831080
6	1.017272	6.015855	3.094183

1	0.030137	6.440503	3.256005
6	2.067725	6.413397	3.919635
1	1.890596	7.137300	4.709493
6	3.604356	4.963813	2.741402
1	4.599778	4.551369	2.596269
6	3.353220	5.892824	3.746720
1	4.159096	6.214094	4.398796
1	0.415249	4.658876	-0.879473
1	-0.180155	2.615462	0.856379
6	3.503421	4.077772	-0.251663
1	4.547544	4.095377	0.082688
1	3.407944	3.396882	-1.100717
1	3.204629	5.079732	-0.562321
6	2.973943	2.271198	1.287308
1	2.292571	1.970905	2.084352
1	2.875346	1.574564	0.451491
1	4.004944	2.246473	1.659751

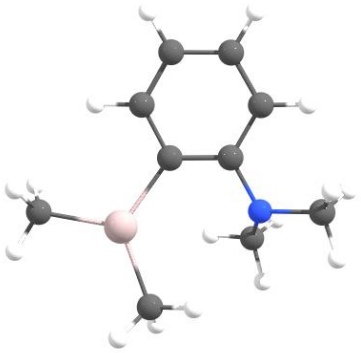

Figure S57: Computed structure of CH_3/CH_3 (FLP)

Data for system: **CH_3/CH_3 (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -687.841581101 A.U.
Zero-point correction= 0.237277 (Hartree/Particle)
Thermal correction to Energy= 0.252058
Thermal correction to Enthalpy= 0.253002
Thermal correction to Gibbs Free Energy= 0.195321
Sum of electronic and zero-point Energies= -687.417906
Sum of electronic and thermal Energies= -687.403126
Sum of electronic and thermal Enthalpies= -687.402181
Sum of electronic and thermal Free Energies= -687.459862

Optimized Geometry (XYZ coordinates in Angstrom)

6	3.082380	4.611482	2.071369
6	1.909546	5.402059	2.026388
13	0.609503	5.414678	0.559459
7	3.482663	3.924984	0.890142
6	1.542679	6.080340	3.197365
1	0.643818	6.695610	3.192670

6	2.268878	5.975493	4.383823
1	1.950634	6.506153	5.275239
6	3.808515	4.491949	3.260454
1	4.705002	3.882885	3.299379
6	3.397251	5.167232	4.408640
1	3.975262	5.063475	5.322235
6	3.927930	4.786589	-0.197929
1	4.956476	5.151687	-0.037180
1	3.895658	4.233789	-1.141808
1	3.275327	5.655749	-0.288849
6	4.394816	2.811459	1.063727
1	4.027237	2.148251	1.849440
1	4.439537	2.247712	0.127568
1	5.423188	3.123288	1.316389
6	0.736259	4.266189	-1.021204
1	1.206562	4.803879	-1.854068
1	1.355168	3.388293	-0.815433
1	-0.244484	3.935812	-1.376410
6	-0.903385	6.643932	0.801935
1	-0.578122	7.645193	1.104670
1	-1.503733	6.749750	-0.106039
1	-1.576685	6.287517	1.591050

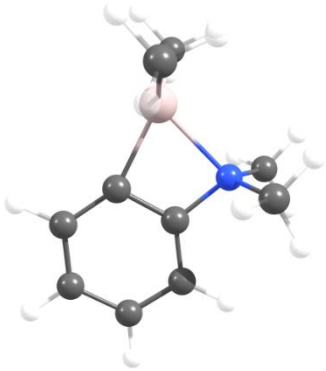

Figure S58: Computed structure of CH_3/CH_3 (CLA)

Data for system: **CH_3/CH_3 (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -687.866664636 A.U.
Zero-point correction= 0.237694 (Hartree/Particle)
Thermal correction to Energy= 0.252102
Thermal correction to Enthalpy= 0.253046
Thermal correction to Gibbs Free Energy= 0.197502

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.914293	5.035880	2.155006
6	1.909844	6.005524	2.130401
13	1.068293	5.226872	0.494384

7	2.760587	4.087680	1.036926
6	1.953492	6.964481	3.148723
1	1.204667	7.751054	3.195182
6	2.953925	6.929478	4.119029
1	2.973978	7.680943	4.902874
6	3.929820	4.964521	3.103418
1	4.689145	4.186728	3.076394
6	3.937237	5.936869	4.099024
1	4.709140	5.923830	4.861912
6	3.895883	4.126360	0.100402
1	4.807446	3.736759	0.569920
1	3.656808	3.520039	-0.776914
1	4.064161	5.157089	-0.214214
6	2.497992	2.712190	1.491497
1	1.655224	2.719765	2.183903
1	2.244592	2.092308	0.627783
1	3.376431	2.288526	1.993544
6	1.445232	6.038147	-1.263484
6	-0.512190	4.062342	0.685142
1	-1.429806	4.596151	0.412722
1	-0.458251	3.189744	0.022535
1	-0.656378	3.689529	1.704752
1	0.597725	6.640634	-1.609710
1	1.614645	5.277239	-2.035342
1	2.319067	6.698293	-1.258754

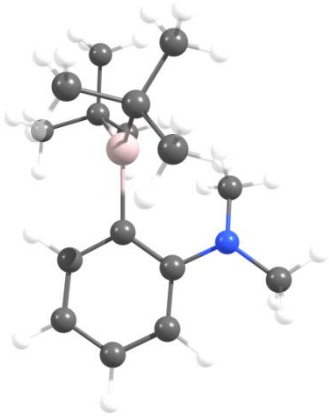

Figure S59: Computed structure of CH3/tbut (FLP)

Data for system: **CH3/tbut (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -923.671617021 A.U.
Zero-point correction= 0.409212 (Hartree/Particle)
Thermal correction to Energy= 0.431710
Thermal correction to Enthalpy= 0.432654
Thermal correction to Gibbs Free Energy= 0.358440

Optimized Geometry (XYZ coordinates in Angstrom)

6	-0.442470	-1.482205	0.661032
6	-0.603414	-1.793554	-0.713233
7	-1.092692	-0.819675	-1.597183
13	-0.672541	0.308332	1.437170
6	0.768166	1.622108	1.053954
6	-2.072664	0.578403	2.825888
6	1.735055	1.557601	2.250273
1	1.258365	1.878780	3.185113
1	2.134517	0.546464	2.405121
1	2.599713	2.219095	2.085559
6	0.287646	3.067739	0.886642
1	-0.219131	3.443023	1.781508
1	1.141001	3.735059	0.689834
1	-0.403496	3.178850	0.041153
6	1.523760	1.195347	-0.211735
1	2.375701	1.867728	-0.396425
1	1.915034	0.175319	-0.129640
6	-1.685663	-0.336519	4.003084
1	-2.408961	-0.225649	4.825759
1	-1.684193	-1.394124	3.715158
1	-0.696571	-0.094719	4.415031
6	-2.147698	2.022758	3.332323
1	-2.889387	2.109143	4.141374
1	-1.188107	2.368857	3.734502
1	-2.445170	2.720825	2.541305
6	-3.458621	0.150299	2.327330
1	-3.456876	-0.875725	1.939945
1	-4.191164	0.188976	3.148275
1	-3.831784	0.811141	1.535098
6	-1.960845	0.206425	-1.065971
1	-2.512279	0.682243	-1.878232
1	-2.695298	-0.190696	-0.350304
1	-1.395798	1.037410	-0.597768
6	-1.284021	-1.174928	-2.988362
1	-0.345892	-1.541962	-3.412614
1	-2.055221	-1.946791	-3.137416
1	-1.570196	-0.283818	-3.548545
6	0.071168	-2.488212	1.492583
1	0.214840	-2.279624	2.553236
6	0.422151	-3.754010	1.025922
1	0.818736	-4.503921	1.701859
6	-0.261068	-3.070186	-1.188453
1	-0.399190	-3.331442	-2.230425
6	0.250338	-4.032116	-0.323263
1	0.506049	-5.011375	-0.716856
1	0.884581	1.222634	-1.103110

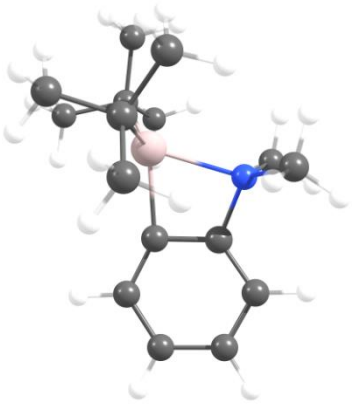

Figure S60: Computed structure of CH3/t-but (CLA)

Data for system: **CH3/t-but (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -923.691761583 A.U.
Zero-point correction= 0.410490 (Hartree/Particle)
Thermal correction to Energy= 0.432271
Thermal correction to Enthalpy= 0.433215
Thermal correction to Gibbs Free Energy= 0.362155

Optimized Geometry (XYZ coordinates in Angstrom)

6	-0.281517	-1.626297	0.772300
6	-0.589588	-1.753300	-0.582844
7	-1.195261	-0.516217	-1.113507
13	-0.790403	0.300227	0.837643
6	0.759218	1.581164	0.741591
6	-2.425191	0.858391	1.859257
6	0.981451	2.172383	2.145259
1	0.134538	2.780572	2.481371
1	1.155777	1.395939	2.901088
1	1.868131	2.826071	2.146462
6	0.532217	2.753941	-0.222556
1	-0.383831	3.309095	0.012300
1	1.367760	3.469878	-0.166174
1	0.465093	2.430401	-1.267113
6	2.058524	0.857844	0.358653
1	2.908224	1.558628	0.372945
1	2.288427	0.044826	1.056274
6	-2.031659	0.679768	3.338913
1	-2.870301	0.964141	3.993905
1	-1.783222	-0.363950	3.569782
1	-1.176069	1.299272	3.627697
6	-2.801908	2.326918	1.625105
1	-3.650053	2.620598	2.263946
1	-1.975783	3.009363	1.853832
1	-3.102007	2.511245	0.585590
6	-3.674672	0.000385	1.625790
1	-3.462779	-1.074110	1.697900

1	-4.440743	0.230546	2.382984
1	-4.131668	0.194178	0.649763
6	-2.609443	-0.730773	-1.477084
1	-3.087256	0.235676	-1.659317
1	-2.682846	-1.345955	-2.382672
1	-3.118653	-1.238803	-0.659796
6	-0.472987	0.028696	-2.276042
1	0.575381	0.176670	-2.020613
1	-0.542905	-0.653251	-3.132266
1	-0.915747	0.988596	-2.552366
6	0.275746	-2.751720	1.389981
1	0.543047	-2.722975	2.443359
6	0.501121	-3.922648	0.668088
1	0.934473	-4.788082	1.160608
6	-0.377707	-2.901430	-1.340244
1	-0.634897	-2.952292	-2.395344
6	0.179492	-3.998304	-0.689414
1	0.363314	-4.915862	-1.239162
1	2.028989	0.414326	-0.642962

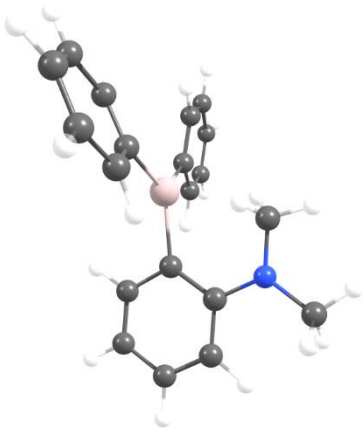

Figure S61: Computed structure of CH3/Ph (FLP)

Data for system: **CH3/Ph (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1071.30955329 A.U.
Zero-point correction= 0.347679 (Hartree/Particle)
Thermal correction to Energy= 0.368602
Thermal correction to Enthalpy= 0.369546
Thermal correction to Gibbs Free Energy= 0.293834

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.460084	5.022945	1.418247
6	1.363873	5.901426	1.619602
13	-0.497438	5.461089	2.006069
7	2.296680	3.642307	1.500370
6	1.618753	7.280853	1.544637

1	0.794973	7.981783	1.692022
6	2.878245	7.811213	1.282530
1	3.031088	8.883674	1.232996
6	3.733986	5.555584	1.137682
1	4.580114	4.902599	0.964116
6	3.932161	6.928465	1.077258
1	4.927101	7.306405	0.861179
6	3.386475	2.774511	1.107081
1	4.259243	2.927441	1.750628
1	3.075347	1.735653	1.216463
1	3.698780	2.935984	0.065060
6	0.968761	3.086580	1.564462
1	0.331181	3.389363	0.715390
1	1.024087	1.998006	1.546710
1	0.469941	3.337882	2.516020
6	-1.081400	5.277684	3.862050
6	-2.298828	4.680915	4.235965
6	-0.240245	5.723547	4.897361
6	-2.663523	4.540997	5.572704
6	-0.599802	5.596241	6.236963
6	-1.814095	5.003943	6.574931
1	-2.975306	4.306048	3.470002
1	0.718335	6.177550	4.650437
1	-3.607612	4.072516	5.834148
1	0.065996	5.953752	7.016661
1	-2.096831	4.899675	7.618113
6	-1.801032	5.419782	0.551275
6	-1.361690	5.262628	-0.775367
6	-3.184137	5.567604	0.755262
6	-2.254223	5.233977	-1.843906
6	-4.085447	5.545230	-0.306593
6	-3.619898	5.372948	-1.607892
1	-0.295173	5.169477	-0.978472
1	-3.567956	5.715597	1.762714
1	-1.887738	5.109634	-2.858416
1	-5.148794	5.663731	-0.121415
1	-4.319988	5.353558	-2.437634

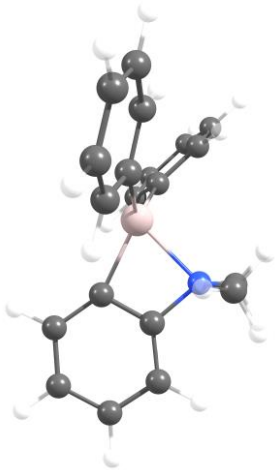

Figure S62: Computed structure of CH3/Ph (CLA)

Data for system: **CH3/Ph (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1071.33541567 A.U.
Zero-point correction= 0.348431 (Hartree/Particle)
Thermal correction to Energy= 0.368661
Thermal correction to Enthalpy= 0.369606
Thermal correction to Gibbs Free Energy= 0.297597

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.335403	5.228999	1.408740
6	1.400731	6.261683	1.512596
13	-0.063498	5.012699	1.996169
7	1.725049	3.929516	1.741301
6	1.861578	7.551293	1.227083
1	1.186872	8.401385	1.283873
6	3.189980	7.765169	0.863282
1	3.536055	8.770932	0.644532
6	3.668209	5.400668	1.048295
1	4.358458	4.563508	0.981992
6	4.088471	6.698589	0.773167
1	5.119096	6.882880	0.487119
6	2.286843	3.346785	2.974567
1	2.234205	4.084792	3.776118
1	1.690237	2.477327	3.261188
1	3.328986	3.042152	2.819991
6	1.779806	2.962234	0.631642
1	2.812058	2.648326	0.435341
1	1.181163	2.086973	0.895126
1	1.358589	3.417025	-0.265480
6	-0.556666	4.759805	3.885347
6	-1.169334	3.576671	4.336907
6	-0.235043	5.715625	4.864388
6	-1.451079	3.357903	5.684027
6	-0.515884	5.512442	6.214489
6	-1.125738	4.330377	6.626383
1	-1.433701	2.797898	3.621321
1	0.251711	6.643665	4.567449
1	-1.924709	2.432687	5.999451
1	-0.258080	6.273306	6.945511
1	-1.345313	4.166773	7.677118
6	-1.331225	4.473496	0.591205
6	-1.050165	4.718532	-0.765204
6	-2.552883	3.841191	0.878053
6	-1.924198	4.339030	-1.781169
6	-3.437386	3.456471	-0.128412
6	-3.120993	3.701565	-1.461821
1	-0.127324	5.231942	-1.036814
1	-2.830608	3.654634	1.914061
1	-1.678245	4.544874	-2.818927
1	-4.374468	2.970066	0.126531
1	-3.807629	3.404598	-2.248902

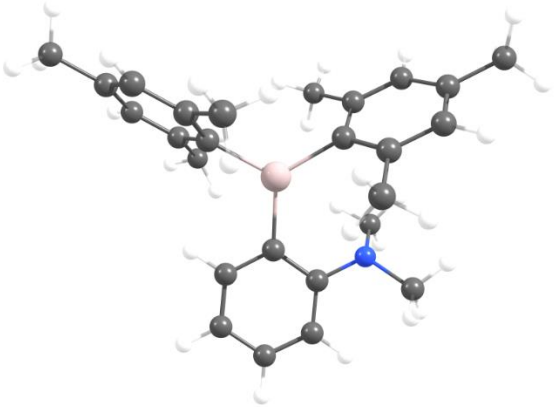

Figure S63: Computed structure of CH3/Mes (FLP)

Data for system: **CH3/Mes (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1307.17472382 A.U.
Zero-point correction= 0.513680 (Hartree/Particle)
Thermal correction to Energy= 0.544621
Thermal correction to Enthalpy= 0.545565
Thermal correction to Gibbs Free Energy= 0.449632

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.465374	4.754247	1.525349
6	1.361514	5.305420	0.831565
13	-0.493697	5.130196	1.434414
7	2.246062	4.230723	2.824972
6	1.588516	5.815525	-0.455307
1	0.750527	6.238566	-1.009480
6	2.842920	5.766811	-1.063078
1	2.986275	6.159874	-2.064234
6	3.720596	4.685745	0.912663
1	4.563817	4.254115	1.442204
6	3.902161	5.187536	-0.374850
1	4.884685	5.131275	-0.834258
6	3.153190	3.205736	3.294473
1	4.131749	3.597982	3.622093
1	2.689671	2.702576	4.149712
1	3.318256	2.466875	2.506456
6	1.946133	5.196067	3.872884
1	1.340165	6.011664	3.473244
1	1.376541	4.708829	4.671529
1	2.865587	5.633743	4.296872
6	-0.982077	4.196726	3.091753
6	-0.645332	2.848653	3.318058
6	-1.568687	4.923398	4.145291
6	-0.875651	2.265628	4.565113
6	-1.795543	4.320438	5.382774
6	-1.452216	2.987905	5.610147
1	-0.601366	1.224425	4.727781

1	-2.238692	4.900943	6.189960
6	-1.871166	5.915667	0.271819
6	-2.808312	5.061089	-0.349369
6	-1.973078	7.297371	0.031188
6	-3.797955	5.579118	-1.178825
6	-2.975062	7.797002	-0.806995
6	-3.895624	6.952440	-1.419110
1	-4.508097	4.904798	-1.654661
1	-3.037323	8.869029	-0.984849
6	-1.723434	2.335793	6.941628
1	-2.708829	1.857933	6.947627
1	-0.982926	1.562953	7.162668
1	-1.708243	3.067954	7.752691
6	-0.055651	2.010117	2.208568
1	-0.844282	1.599172	1.567049
1	0.624394	2.600263	1.582920
1	0.516004	1.165704	2.603898
6	-1.907568	6.385740	3.954351
1	-0.996013	6.989903	3.840693
1	-2.521031	6.539946	3.058835
1	-2.453031	6.791903	4.809416
6	-1.031816	8.269713	0.706600
1	-0.974642	9.217015	0.164563
1	-1.370575	8.498711	1.724300
1	-0.014612	7.867260	0.776712
6	-2.725150	3.567301	-0.121115
1	-2.810498	3.324723	0.945218
1	-3.515916	3.030800	-0.650659
1	-1.767438	3.164870	-0.477832
6	-4.976538	7.492859	-2.319707
1	-4.927177	7.034494	-3.311982
1	-5.969412	7.278763	-1.912023
1	-4.887862	8.574621	-2.441209

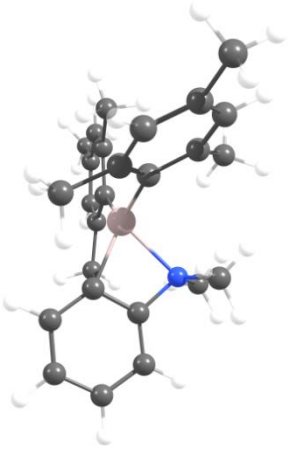

Figure S64: Computed structure of CH3/Mes (CLA)

Data for system: **CH3/Mes (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1307.18972909 A.U.
Zero-point correction= 0.515499 (Hartree/Particle)
Thermal correction to Energy= 0.545548
Thermal correction to Enthalpy= 0.546492
Thermal correction to Gibbs Free Energy= 0.454269

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.626332	4.930448	1.330335
6	1.837409	5.462506	0.309227
13	0.126164	5.106354	1.261986
7	1.790702	4.327416	2.384613
6	2.514958	6.042965	-0.767190
1	1.959038	6.476747	-1.595243
6	3.908587	6.083006	-0.790687
1	4.423912	6.540232	-1.630135
6	4.017084	4.952327	1.346014
1	4.591267	4.527850	2.165695
6	4.656007	5.547001	0.260805
1	5.740031	5.591322	0.231591
6	1.941591	2.856463	2.361110
1	2.970513	2.581204	2.623199
1	1.253314	2.409802	3.080343
1	1.703682	2.484356	1.364413
6	2.067886	4.832500	3.740522
1	1.979601	5.917714	3.756718
1	1.334409	4.404833	4.428738
1	3.072913	4.543994	4.071607
6	-0.835198	6.627368	2.142090
6	-0.184252	7.753874	2.694882
6	-2.255889	6.604353	2.252602
6	-0.900097	8.736866	3.391582
6	-2.939594	7.601787	2.942647
6	-2.275675	8.671241	3.544777
1	-0.358176	9.584765	3.808779
1	-4.025472	7.553937	3.004299
6	-0.830445	3.427370	0.798031
6	-0.958589	3.011509	-0.547621
6	-1.333892	2.567172	1.790765
6	-1.544355	1.788095	-0.863530
6	-1.913200	1.338698	1.453380
6	-2.022372	0.929679	0.129739
1	-1.637140	1.492384	-1.907587
1	-2.296907	0.693666	2.243032
6	-3.038134	9.718436	4.313708
1	-3.405163	9.315874	5.263516
1	-2.409172	10.583166	4.537359
1	-3.908992	10.065335	3.750172
6	1.296081	8.040431	2.539971
1	1.781921	8.158503	3.515550
1	1.832698	7.281143	1.974273
1	1.432705	8.987561	2.007820
6	-3.105847	5.536318	1.595887
1	-2.812227	5.357593	0.557949
1	-3.035723	4.573313	2.107490
1	-4.156463	5.836689	1.598052
6	-1.317582	2.944771	3.259211

1	-2.336751	3.049937	3.646878
1	-0.830612	2.175998	3.869708
1	-0.811462	3.899248	3.442575
6	-0.463060	3.892942	-1.674095
1	0.630992	3.904879	-1.720636
1	-0.840312	3.550368	-2.640833
1	-0.786877	4.932664	-1.542291
6	-2.642239	-0.394536	-0.236594
1	-3.464490	-0.261457	-0.946020
1	-1.908800	-1.054606	-0.710535
1	-3.035094	-0.906129	0.645007

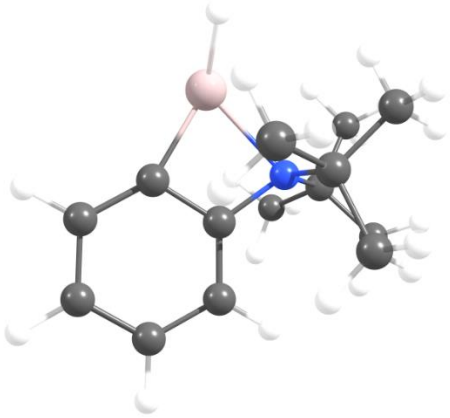

Figure S65: Computed structure of t-but/H (CLA)

Data for system: **t-but/H (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -845.047556986 A.U.
Zero-point correction= 0.351416 (Hartree/Particle)
Thermal correction to Energy= 0.368698
Thermal correction to Enthalpy= 0.369642
Thermal correction to Gibbs Free Energy= 0.309490

Optimized Geometry (XYZ coordinates in Angstrom)

6	0.094984	-0.996965	2.484117
6	1.278509	-0.675377	3.150602
1	1.865162	-1.465021	3.610375
1	-0.236015	-2.029541	2.434951
6	-0.669800	-0.001193	1.882053
6	1.697318	0.650318	3.240451
1	2.610683	0.880839	3.782480
6	0.951966	1.673689	2.649220
6	-0.214741	1.314793	1.967108
1	-1.596086	-0.256959	1.377653
7	-0.866087	2.499944	1.357748
13	0.641466	3.615482	2.455892

1	0.020480	4.315378	3.742479
1	1.432889	4.610307	1.502102
6	-0.631900	2.498082	-0.169588
6	-2.274750	2.802683	1.913921
6	-3.435260	2.139116	1.161213
1	-3.587015	2.559789	0.165377
1	-3.314149	1.056598	1.080370
1	-4.349540	2.324593	1.732346
6	-2.527260	4.321243	1.936795
1	-1.756053	4.848144	2.503652
1	-2.603477	4.762619	0.945696
1	-3.479547	4.499646	2.444415
6	-2.347449	2.314775	3.373360
1	-3.280529	2.687056	3.803838
1	-2.352086	1.226119	3.442895
1	-1.523782	2.699741	3.977335
6	-1.302282	1.339207	-0.931423
1	-1.037928	1.451687	-1.987015
1	-0.912708	0.372884	-0.606998
1	-2.387199	1.325839	-0.873444
6	0.875936	2.338761	-0.450353
1	1.262404	1.387185	-0.081773
1	1.012571	2.359951	-1.534785
1	1.467424	3.151104	-0.027765
6	-1.073753	3.830542	-0.779702
1	-0.700578	3.879320	-1.806085
1	-2.159768	3.930624	-0.827057
1	-0.653051	4.676916	-0.229325

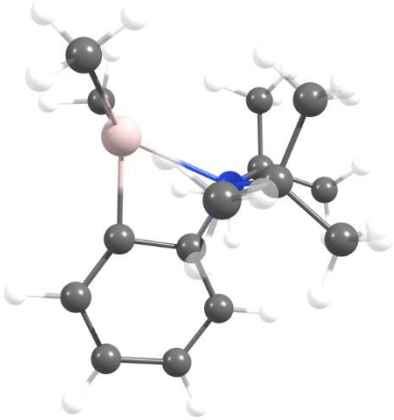

Figure S66: Computed structure of t-but/CH3 (CLA)

Data for system: **t-but/CH3 (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -923.690098817 A.U.
Zero-point correction= 0.409812 (Hartree/Particle)
Thermal correction to Energy= 0.431155
Thermal correction to Enthalpy= 0.432099

Thermal correction to Gibbs Free Energy= 0.363331

Optimized Geometry (XYZ coordinates in Angstrom)

6	-0.209632	-1.071253	2.772504
6	1.079619	-0.913968	3.281762
1	1.550984	-1.736284	3.811695
1	-0.738894	-2.008347	2.914239
6	-0.827792	-0.029696	2.084972
6	1.750900	0.297397	3.127766
1	2.745142	0.406491	3.553789
6	1.158539	1.364007	2.444141
6	-0.122444	1.163125	1.919860
1	-1.839247	-0.152855	1.710894
7	-0.608454	2.352071	1.185889
13	1.303853	3.290307	2.001001
6	-0.574290	2.085070	-0.331182
6	-1.860405	3.001098	1.806553
6	-3.208319	2.528813	1.243289
1	-3.384753	2.870851	0.221780
1	-3.317025	1.442761	1.282949
1	-3.996069	2.959951	1.868242
6	-1.791868	4.530206	1.651750
1	-0.893888	4.938074	2.119340
1	-1.828686	4.858438	0.615038
1	-2.654151	4.969344	2.162016
6	-1.889568	2.694977	3.315825
1	-2.625387	3.355809	3.781641
1	-2.183693	1.663362	3.515841
1	-0.926043	2.870246	3.792688
6	-1.562045	1.019672	-0.848979
1	-1.359618	0.886073	-1.915827
1	-1.393830	0.053090	-0.371685
1	-2.610294	1.289585	-0.756540
6	0.816259	1.540880	-0.711321
1	1.006617	0.566196	-0.258426
1	0.841526	1.419233	-1.797445
1	1.623232	2.217013	-0.436949
6	-0.799690	3.386556	-1.105812
1	-0.553560	3.213500	-2.156938
1	-1.838944	3.719531	-1.069010
1	-0.154240	4.186635	-0.734894
6	2.523756	4.092304	0.657253
1	3.041889	4.931463	1.136462
1	3.295997	3.396419	0.310106
1	2.043340	4.498530	-0.239676
6	1.131808	4.566337	3.507488
1	2.101209	4.515859	4.025269
1	1.042244	5.600442	3.153267
1	0.367116	4.412944	4.272356

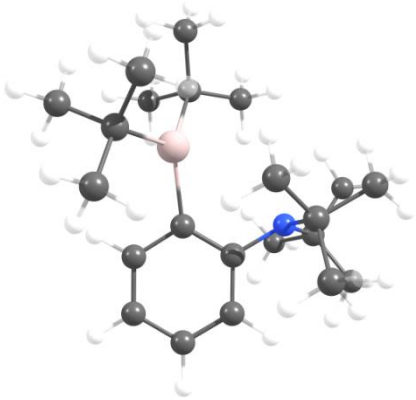

Figure S67: Computed structure of t-but/t-but (FLP)

Data for system: **t-but/t-but (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1159.50235062 A.U.
Zero-point correction= 0.580410 (Hartree/Particle)
Thermal correction to Energy= 0.609917
Thermal correction to Enthalpy= 0.610861
Thermal correction to Gibbs Free Energy= 0.524279

Optimized Geometry (XYZ coordinates in Angstrom)

6	-3.857837	-0.840354	0.630990
6	-3.268612	-1.148489	1.872583
13	-1.619685	-2.208186	2.104875
7	-3.064755	-0.934660	-0.585400
6	-4.034824	-0.931191	3.032581
1	-3.604412	-1.160951	4.008227
6	-5.335211	-0.438832	2.992562
1	-5.888260	-0.263448	3.909963
6	-5.196145	-0.422095	0.590262
1	-5.673957	-0.248523	-0.366783
6	-5.925457	-0.207717	1.754992
1	-6.952835	0.137353	1.690774
6	-1.900795	-3.935104	3.082921
6	0.224535	-1.476811	1.965602
6	1.337662	-2.527470	2.034335
6	0.336324	-0.552798	3.195160
6	0.433457	-0.630809	0.710009
6	-1.171401	-5.097028	2.391142
6	-1.307167	-3.761376	4.493938
6	-3.375591	-4.325793	3.242031
1	-0.235638	-3.532246	4.473514
1	-1.427251	-4.687928	5.076587
1	-1.272565	-6.018972	2.984770
1	-0.099993	-4.907092	2.268647
1	-1.589359	-5.308643	1.399298
1	-3.957139	-3.562087	3.767504
1	-3.868615	-4.502802	2.279258

1	-3.457695	-5.259777	3.819229
1	0.397149	-1.244039	-0.198724
1	1.417509	-0.136680	0.733874
1	2.323405	-2.036998	2.034785
1	1.282429	-3.140285	2.940195
1	1.313459	-3.205355	1.172961
1	0.229211	-1.099265	4.141078
1	1.323047	-0.065007	3.217935
1	-0.328438	0.148911	0.613935
1	-1.806757	-2.963614	5.059470
1	-0.416603	0.245578	3.178833
6	-3.247006	-2.240794	-1.293595
6	-2.938589	0.365582	-1.341470
6	-4.714500	-2.580502	-1.622913
1	-4.761811	-3.533446	-2.159274
1	-5.314443	-2.676083	-0.715110
1	-5.169821	-1.815649	-2.257115
6	-2.708745	-3.351046	-0.373690
1	-3.285931	-3.429075	0.550704
1	-2.763484	-4.325142	-0.869030
1	-1.641804	-3.167850	-0.158583
6	-2.427842	-2.347332	-2.585111
1	-1.370879	-2.139212	-2.404791
1	-2.512649	-3.372773	-2.955514
1	-2.792177	-1.689587	-3.374938
6	-2.910426	1.518232	-0.317933
1	-2.147298	1.339990	0.445325
1	-2.666051	2.445633	-0.841778
1	-3.865188	1.660048	0.188928
6	-1.592533	0.451570	-2.098033
1	-0.785772	0.021548	-1.505965
1	-1.613337	-0.035649	-3.071677
1	-1.357614	1.504000	-2.280431
6	-4.052866	0.668967	-2.363728
1	-3.817534	1.611744	-2.868884
1	-4.127128	-0.100380	-3.135738
1	-5.032382	0.789286	-1.897454

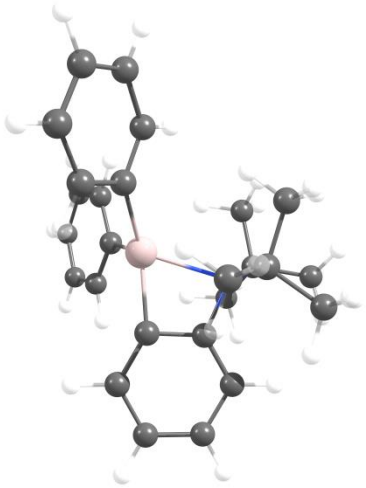

Figure S68: Computed structure of t-but/Ph (CLA)

Data for system: **t-but/Ph (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1307.15853194 A.U.
Zero-point correction= 0.519882 (Hartree/Particle)
Thermal correction to Energy= 0.547212
Thermal correction to Enthalpy= 0.548156
Thermal correction to Gibbs Free Energy= 0.464075

Optimized Geometry (XYZ coordinates in Angstrom)

6	-0.636513	-1.129186	2.937741
6	0.728501	-1.376342	2.784894
1	1.128199	-2.352979	3.040633
1	-1.289520	-1.908858	3.317040
6	-1.169611	0.115073	2.611704
6	1.576998	-0.370264	2.327414
1	2.641880	-0.572378	2.244619
6	1.073025	0.889403	1.989237
6	-0.304078	1.097029	2.128514
1	-2.229554	0.306355	2.748856
7	-0.698519	2.450596	1.679864
13	1.510411	2.784471	1.662575
6	-1.344981	2.352142	0.274604
6	-1.381414	3.323276	2.751275
6	-2.916676	3.303109	2.754690
1	-3.357451	3.776018	1.875998
1	-3.313828	2.290369	2.853908
1	-3.249507	3.870664	3.628415
6	-0.907273	4.778494	2.589967
1	0.163954	4.866383	2.794883
1	-1.115523	5.192633	1.605133
1	-1.422653	5.401102	3.327228
6	-0.942306	2.862872	4.151867
1	-1.259837	3.625433	4.868134
1	-1.403752	1.916243	4.437222
1	0.139352	2.763008	4.239141
6	-2.686393	1.593425	0.229148
1	-2.970216	1.507864	-0.823711
1	-2.585515	0.577165	0.613074
1	-3.506464	2.091505	0.738865
6	-0.412248	1.557343	-0.659822
1	-0.296315	0.520857	-0.338694
1	-0.867923	1.553730	-1.653475
1	0.571604	2.014153	-0.759051
6	-1.533246	3.740538	-0.342817
1	-1.862502	3.609364	-1.377153
1	-2.297630	4.331678	0.164126
1	-0.593250	4.296942	-0.363700
6	2.132956	3.729913	0.037572
6	2.947792	3.079206	-0.905098
6	1.907272	5.101854	-0.174468
6	3.499939	3.748428	-1.996041
6	2.445299	5.782889	-1.264829
6	3.246469	5.104777	-2.179648
1	3.155369	2.014902	-0.794328

1	1.287337	5.663369	0.525600
1	4.125645	3.212034	-2.703407
1	2.243171	6.841565	-1.399185
1	3.670979	5.630484	-3.029407
6	2.379876	3.567755	3.268184
6	2.659877	2.766369	4.389838
6	2.880864	4.880932	3.297818
6	3.374790	3.247169	5.485115
6	3.591426	5.378075	4.388801
6	3.837852	4.560308	5.488464
1	2.306303	1.735337	4.410208
1	2.726370	5.534571	2.440693
1	3.572491	2.598957	6.334064
1	3.959885	6.399848	4.378418
1	4.394416	4.941655	6.339363

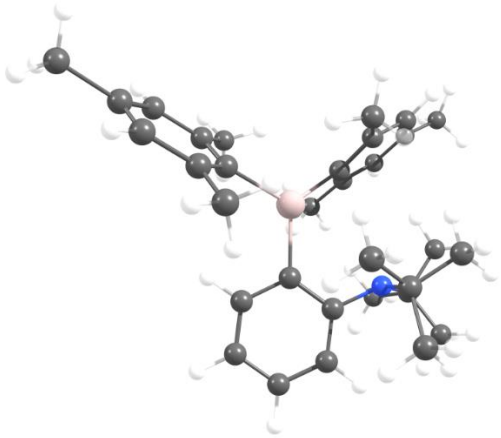

Figure S69: Computed structure of t-but/Mes

Data for system: **t-but/Mes**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1543.00896388 A.U.
Zero-point correction= 0.685557 (Hartree/Particle)
Thermal correction to Energy= 0.723138
Thermal correction to Enthalpy= 0.724083
Thermal correction to Gibbs Free Energy= 0.617562

Optimized Geometry (XYZ coordinates in Angstrom)

6	-3.637781	-0.339001	-2.614194
6	-3.791930	-0.623010	-1.240943
13	-2.612919	0.008664	0.198651
7	-2.514943	0.464857	-3.050873
6	-4.870342	-1.436806	-0.849685
1	-4.981935	-1.697814	0.203035
6	-5.795208	-1.933981	-1.764345
1	-6.623290	-2.551470	-1.430723
6	-4.562341	-0.854430	-3.531697
1	-4.442750	-0.637875	-4.588310

6	-5.637777	-1.634017	-3.112844
1	-6.344081	-2.013429	-3.845158
6	-1.403007	-0.362919	-3.612478
6	-2.865635	1.809179	-3.631257
6	-1.745102	-1.142440	-4.901264
1	-0.851612	-1.670620	-5.250011
1	-2.517728	-1.892235	-4.716020
1	-2.080988	-0.489483	-5.708223
6	-1.013150	-1.410395	-2.558880
1	-1.823073	-2.113559	-2.359292
1	-0.144481	-1.979859	-2.903321
1	-0.734894	-0.915217	-1.620316
6	-0.146907	0.478730	-3.867466
1	0.687515	-0.196399	-4.078570
1	-0.251022	1.140448	-4.729129
1	0.103677	1.078970	-2.988688
6	-4.188606	2.276038	-3.001141
1	-4.112507	2.254050	-1.912586
1	-4.382005	3.305885	-3.312117
1	-5.041336	1.664489	-3.300145
6	-1.817426	2.873888	-3.234046
1	-1.498965	2.730233	-2.200071
1	-0.939381	2.872599	-3.879347
1	-2.268482	3.867800	-3.316702
6	-3.039069	1.851080	-5.160578
1	-2.110761	1.623352	-5.689561
1	-3.816194	1.164108	-5.506958
1	-3.338276	2.862823	-5.454078
6	-1.771044	1.785991	0.247897
6	-0.371563	1.930369	0.161030
6	0.547867	0.727862	0.170754
1	0.874718	0.458187	-0.839796
1	0.068475	-0.152117	0.617868
1	1.447949	0.930256	0.757805
6	0.204300	3.198108	0.056997
1	1.286904	3.288396	-0.017903
6	-0.576098	4.353081	0.050326
1	-0.509970	6.478967	0.421052
6	0.051462	5.712561	-0.119061
1	1.082131	5.722128	0.243590
1	0.069820	6.000736	-1.175524
1	-2.578501	5.107905	0.228385
6	-1.955966	4.215096	0.193964
6	-2.553686	2.958884	0.297949
6	-4.047003	2.901334	0.535261
1	-4.480507	1.929462	0.264818
1	-4.275632	3.077075	1.592249
1	-4.576208	3.661786	-0.046015
6	-2.493212	-1.168082	1.788391
6	-2.833588	-0.659704	3.062493
6	-3.337992	0.757595	3.220688
1	-3.506199	1.005173	4.271413
1	-4.293992	0.893910	2.699918
1	-2.630649	1.485764	2.809661
6	-2.746146	-1.464050	4.198515
1	-3.020418	-1.050090	5.167120
6	-2.321756	-2.789123	4.121475
1	-1.221213	-3.490798	5.835594
6	-2.198055	-3.635368	5.361990
1	-2.961444	-3.372571	6.098677

1	-2.297339	-4.698144	5.128407
1	-1.674884	-4.336508	2.784059
6	-1.997082	-3.300224	2.867512
6	-2.078099	-2.515320	1.716139
6	-1.705329	-3.140326	0.391891
1	-1.508713	-4.209847	0.496991
1	-2.507690	-3.014948	-0.342774
1	-0.800137	-2.683048	-0.025611

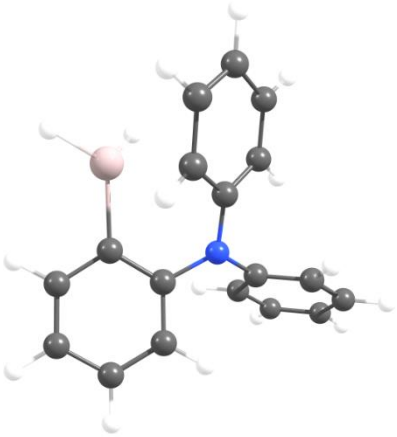

Figure S70: Computed structure of Ph/H (FLP)

Data for system: **Ph/H (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -992.683012459 A.U.
Zero-point correction= 0.285211 (Hartree/Particle)
Thermal correction to Energy= 0.301801
Thermal correction to Enthalpy= 0.302745
Thermal correction to Gibbs Free Energy= 0.240757

Optimized Geometry (XYZ coordinates in Angstrom)

6	-3.035517	3.112044	2.036438
6	-2.498245	4.291883	2.555279
7	-2.273484	1.906746	2.040928
6	-3.256021	5.457859	2.548860
1	-2.834052	6.371504	2.954679
6	-4.542852	5.459982	2.014812
1	-5.128873	6.372829	2.008075
6	-4.329299	3.108987	1.511146
1	-4.737071	2.182328	1.118760
6	-5.074426	4.283272	1.492582
1	-6.078590	4.274163	1.081301
6	-1.569829	1.554357	3.244569
6	-0.254214	1.060650	3.185679
6	0.361591	0.780623	4.412973
1	1.373751	0.379694	4.417047
1	0.241934	0.765400	6.566424

6	-0.272088	0.989254	5.637162
6	-1.576443	1.471756	5.654148
1	-2.093934	1.625095	6.595886
1	-3.253250	2.115385	4.463557
6	-2.232482	1.745595	4.459269
6	-1.979634	1.289325	0.828542
6	-1.565853	-0.064145	0.794239
1	-1.636978	-0.663792	1.696927
6	-1.187347	-0.663112	-0.417436
1	-0.865192	-1.699441	-0.404894
1	-0.915068	-0.407620	-2.536447
6	-1.222842	0.051901	-1.604843
6	-1.672933	1.374689	-1.575195
1	-1.709392	1.949838	-2.495056
1	-2.347180	3.030392	-0.391878
6	-2.040020	1.991615	-0.390857
13	0.632593	0.587841	1.469963
1	-1.493373	4.279864	2.965381
1	1.063187	1.696492	0.425188
1	1.393423	-0.805428	1.519342

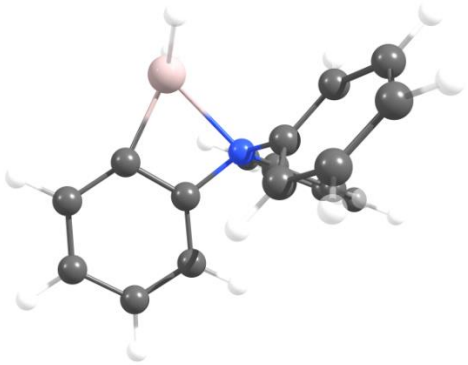

Figure S71: Computed structure of Ph/H (CLA)

Data for system: **Ph/H (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -992.680873596 A.U.
Zero-point correction= 0.285208 (Hartree/Particle)
Thermal correction to Energy= 0.301825
Thermal correction to Enthalpy= 0.302769
Thermal correction to Gibbs Free Energy= 0.240111

Optimized Geometry (XYZ coordinates in Angstrom)

6	-2.248627	3.055452	1.492431
6	-1.204437	3.980226	1.476800
7	-1.940914	1.673275	1.854400
6	-1.466896	5.312449	1.182236
1	-0.648325	6.024216	1.165394

6	-2.766650	5.732143	0.907405
1	-2.967111	6.772276	0.673677
6	-3.554051	3.470975	1.236484
1	-4.368787	2.756128	1.262832
6	-3.805486	4.808746	0.939256
1	-4.823643	5.124965	0.737439
6	-1.475360	1.560795	3.254212
6	-0.243532	0.916593	3.342181
6	0.281871	0.751618	4.628784
1	1.240048	0.259455	4.771766
1	0.012730	1.094556	6.734955
6	-0.407365	1.226172	5.742320
6	-1.631701	1.886946	5.599558
1	-2.149320	2.263314	6.476010
1	-3.129634	2.590072	4.197092
6	-2.186181	2.069155	4.337448
6	-2.947238	0.702315	1.444265
6	-3.587906	-0.136307	2.348547
1	-3.366841	-0.071005	3.407041
6	-4.507133	-1.076106	1.878459
1	-5.001270	-1.731754	2.587796
1	-5.504074	-1.909386	0.165772
6	-4.788967	-1.176306	0.523060
6	-4.136807	-0.334180	-0.378858
1	-4.337887	-0.411431	-1.442105
1	-2.694105	1.247778	-0.619774
6	-3.214922	0.595717	0.076174
13	-0.012706	0.745160	1.381632
1	-0.193748	3.652024	1.694833
1	0.872480	1.833907	0.637699
1	-0.303563	-0.630550	0.653813

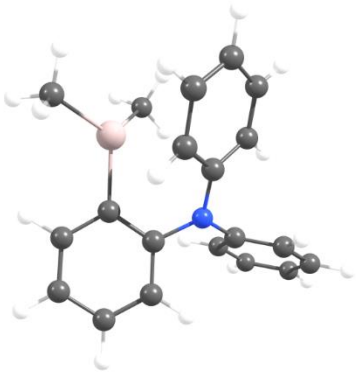

Figure S72: Computed structure of Ph/CH3 (FLP)

Data for system: **Ph/CH3 (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1071.33454455 A.U.
Zero-point correction= 0.343406 (Hartree/Particle)
Thermal correction to Energy= 0.364190
Thermal correction to Enthalpy= 0.365134
Thermal correction to Gibbs Free Energy= 0.293782

Optimized Geometry (XYZ coordinates in Angstrom)

6	-1.639713	4.133724	1.525243
6	-0.524195	4.875398	1.919955
7	-1.669065	2.722535	1.720192
6	-0.508122	6.253553	1.734394
1	0.361035	6.824475	2.044503
6	-1.592811	6.898158	1.143815
1	-1.574516	7.972785	0.996705
6	-2.733403	4.779678	0.944697
1	-3.597810	4.192252	0.650233
6	-2.702578	6.156020	0.746493
1	-3.555189	6.650939	0.292869
6	-1.261286	2.212777	3.001644
6	-0.401367	1.103142	3.084771
6	-0.034188	0.698538	4.375743
1	0.619781	-0.164465	4.493630
1	-0.158122	1.016626	6.506030
6	-0.471699	1.357536	5.524417
6	-1.322963	2.450313	5.399505
1	-1.684647	2.969308	6.281581
1	-2.399513	3.721962	4.031232
6	-1.728707	2.874869	4.138809
6	-1.822367	1.881991	0.620327
6	-2.185286	0.526889	0.794379
1	-2.485277	0.178429	1.777440
6	-2.266790	-0.336662	-0.306486
1	-2.538920	-1.373180	-0.132651
1	-2.059955	-0.553617	-2.438197
6	-2.006504	0.118695	-1.590019
6	-1.683168	1.467134	-1.766474
1	-1.476318	1.844825	-2.763075
1	-1.292884	3.366923	-0.855736
6	-1.582908	2.335988	-0.692595
13	0.156745	0.063705	1.480700
1	0.316128	4.361946	2.376964
6	1.331064	0.892294	0.144244
1	2.367877	0.562405	0.277427
1	1.039135	0.620481	-0.876352
1	1.322528	1.985389	0.207498
6	0.071799	-1.888910	1.704531
1	-0.847450	-2.208909	2.207794
1	0.127275	-2.415164	0.745705
1	0.906251	-2.256205	2.313972

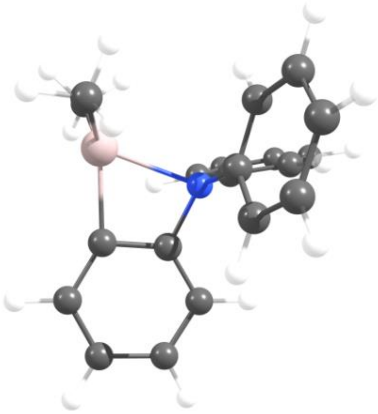

Figure S73: Computed structure of Ph/CH3 (CLA)

Data for system: **Ph/CH3 (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1071.33143154 A.U.
Zero-point correction= 0.343723 (Hartree/Particle)
Thermal correction to Energy= 0.364332
Thermal correction to Enthalpy= 0.365276
Thermal correction to Gibbs Free Energy= 0.294411

Optimized Geometry (XYZ coordinates in Angstrom)

6	-1.242318	3.814563	1.102559
6	0.078137	4.254256	1.221624
7	-1.560712	2.475780	1.578862
6	0.425112	5.532373	0.804457
1	1.455294	5.860001	0.896706
6	-0.538012	6.387286	0.271795
1	-0.263632	7.383992	-0.056628
6	-2.213893	4.673357	0.591224
1	-3.245098	4.348674	0.516052
6	-1.854459	5.953333	0.172741
1	-2.618066	6.613032	-0.226333
6	-1.217046	2.291122	3.001919
6	-0.354594	1.215091	3.205633
6	0.020669	0.965885	4.531833
1	0.692519	0.144115	4.765768
1	-0.143100	1.565019	6.591787
6	-0.446558	1.769795	5.569408
6	-1.293573	2.851409	5.309876
1	-1.639711	3.477353	6.126142
1	-2.336926	3.973149	3.774698
6	-1.689877	3.131068	4.006542
6	-2.851410	1.956242	1.164588
6	-3.810253	1.526513	2.075449
1	-3.627521	1.609697	3.140043
6	-4.998902	0.963092	1.607983
1	-5.739437	0.623045	2.324462

1	-6.161426	0.393913	-0.109206
6	-5.236308	0.834698	0.246149
6	-4.270039	1.268151	-0.662774
1	-4.436751	1.162259	-1.729608
1	-2.315894	2.141573	-0.909114
6	-3.081670	1.818877	-0.208461
13	-0.147810	0.735306	1.286318
1	0.824193	3.593369	1.649826
6	1.415858	1.361997	0.262549
1	1.879677	0.518586	-0.261487
1	1.125991	2.087920	-0.506897
1	2.194400	1.833775	0.870330
6	-1.175867	-0.774485	0.560221
1	-2.153974	-0.892661	1.037765
1	-1.347841	-0.676392	-0.517429
1	-0.626152	-1.712540	0.707482

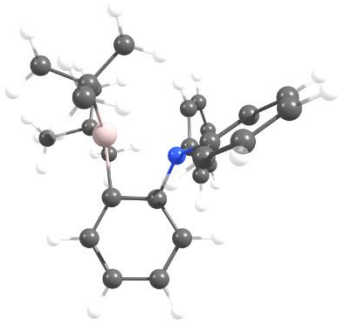

Figure S74: Computed structure of Ph/t-but (FLP)

Data for system: **Ph/t-but (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1307.15852627 A.U.
Zero-point correction= 0.520093 (Hartree/Particle)
Thermal correction to Energy= 0.547339
Thermal correction to Enthalpy= 0.548283
Thermal correction to Gibbs Free Energy= 0.464566

Optimized Geometry (XYZ coordinates in Angstrom)

6	-1.391908	4.128578	1.086547
6	-0.215876	4.657044	1.631071
13	0.857799	3.023646	1.370855
7	-1.301759	2.661988	0.915228
6	-0.182638	6.029490	1.896612
1	0.714113	6.484000	2.310064
6	-1.288077	6.833199	1.625513
1	-1.254860	7.897245	1.839257
6	-2.501324	4.917368	0.779906
1	-3.392044	4.496256	0.323681
6	-2.436962	6.280130	1.058059
1	-3.286904	6.914520	0.827115
6	1.600622	1.717284	2.660427

6	2.002504	2.122876	3.944961
6	1.879886	0.383756	2.311543
6	2.637715	1.255290	4.831940
6	2.506588	-0.497916	3.190289
6	2.889042	-0.061158	4.455823
1	1.809624	3.144487	4.272352
1	1.596637	0.010891	1.326438
1	2.934698	1.605230	5.816292
1	2.699561	-1.523009	2.887576
1	3.380268	-0.742385	5.143801
6	2.129997	3.279110	-0.133880
6	3.081072	2.311061	-0.500886
6	2.214843	4.519629	-0.791700
6	4.039335	2.549788	-1.484226
6	3.171664	4.775544	-1.771892
6	4.084368	3.785077	-2.125122
1	3.086545	1.345260	0.002094
1	1.509494	5.309607	-0.533148
1	4.755574	1.776008	-1.745315
1	3.207117	5.745937	-2.258757
1	4.831262	3.977276	-2.889594
6	-2.092174	1.967560	2.053052
6	-1.484652	2.157956	-0.529861
6	-3.615383	2.204646	2.023482
1	-4.128303	1.753418	1.178709
1	-4.028060	1.748432	2.927893
1	-3.856751	3.267773	2.067247
6	-1.819557	0.461036	2.072293
1	-2.247467	-0.060080	1.214348
1	-0.748857	0.251940	2.131590
1	-2.287771	0.043608	2.967826
6	-1.632798	2.533685	3.410671
1	-2.168314	1.988444	4.192311
1	-0.568164	2.386915	3.588095
1	-1.871705	3.593320	3.515105
6	-1.094223	3.268789	-1.519620
1	-0.124513	3.710209	-1.290849
1	-1.023583	2.819498	-2.513843
1	-1.839005	4.065159	-1.559188
6	-0.522946	0.981789	-0.775867
1	-0.670291	0.153242	-0.085532
1	-0.682343	0.601560	-1.789185
1	0.519294	1.310390	-0.721386
6	-2.905451	1.720747	-0.914123
1	-2.900557	1.497251	-1.984795
1	-3.235080	0.818022	-0.397999
1	-3.637697	2.514720	-0.751048

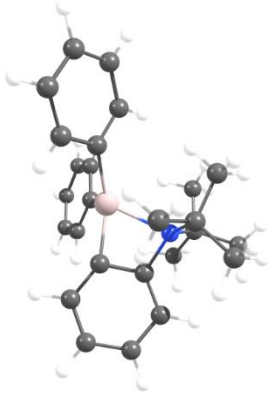

Figure S75: Computed structure of Ph/t-but (CLA)

Data for system: **Ph/t-but (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1307.15672061 A.U.
Zero-point correction= 0.516188 (Hartree/Particle)
Thermal correction to Energy= 0.544357
Thermal correction to Enthalpy= 0.545302
Thermal correction to Gibbs Free Energy= 0.459645

Optimized Geometry (XYZ coordinates in Angstrom)

6	-1.412373	4.225715	1.223188
6	-0.100491	4.655923	1.416063
7	0.886142	3.572230	1.264712
13	-1.048987	2.293000	0.944140
6	0.260816	5.980560	1.657368
1	1.305264	6.269357	1.743199
6	-0.759326	6.920072	1.756418
1	-0.518093	7.960728	1.947855
6	-2.413618	5.200018	1.333672
1	-3.457445	4.927915	1.198413
6	-2.092048	6.528351	1.601193
1	-2.879152	7.272474	1.677758
6	1.449120	3.042834	2.495402
6	1.575629	3.802496	3.654250
6	1.845602	1.703093	2.494854
6	2.099504	3.218408	4.806872
6	2.379469	1.131412	3.642686
6	2.505933	1.888945	4.806475
1	1.241582	4.832594	3.670914
1	1.731837	1.117469	1.584536
1	2.183345	3.812557	5.710815
1	2.679501	0.088672	3.631646
1	2.909702	1.440644	5.707845
6	1.850205	3.817049	0.202100
6	3.173631	3.376949	0.274755
6	1.429738	4.516392	-0.935116
6	4.044917	3.606355	-0.788335

6	2.307870	4.737933	-1.988560
6	3.621250	4.280421	-1.926574
1	3.538628	2.862837	1.154002
1	0.413558	4.889257	-0.992651
1	5.068746	3.254931	-0.711515
1	1.956302	5.275895	-2.862973
1	4.304671	4.454574	-2.750407
6	-1.624138	1.208773	2.530562
6	-0.935363	1.400139	-0.847874
6	-3.155270	1.186731	2.323752
1	-3.455120	0.661402	1.409931
1	-3.643611	0.670938	3.164973
1	-3.577967	2.200178	2.287122
6	-1.123543	-0.236228	2.613528
1	-1.319090	-0.805470	1.698326
1	-0.046379	-0.279898	2.809358
1	-1.622285	-0.770112	3.438012
6	-1.365212	1.891808	3.879408
1	-1.964464	1.407830	4.666998
1	-0.316523	1.819164	4.182567
1	-1.639903	2.953922	3.866704
6	-1.016293	2.359216	-2.042338
1	-0.129701	2.991948	-2.121886
1	-1.088532	1.788065	-2.981435
1	-1.895190	3.012762	-1.989617
6	0.378334	0.607409	-0.938144
1	0.462747	-0.136904	-0.134647
1	0.436074	0.057566	-1.890814
1	1.258108	1.262981	-0.891893
6	-2.103717	0.408903	-0.987752
1	-2.028718	-0.125035	-1.947999
1	-2.115811	-0.348784	-0.197768
1	-3.076740	0.915441	-0.979149

Figure S76: Computed structure of Ph/Ph (FLP)

Data for system: **Ph/Ph (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1454.80348261 A.U.

Zero-point correction= 0.453645 (Hartree/Particle)
Thermal correction to Energy= 0.480394
Thermal correction to Enthalpy= 0.481338
Thermal correction to Gibbs Free Energy= 0.393917

Optimized Geometry (XYZ coordinates in Angstrom)

6	-1.526782	4.512967	1.533937
6	-0.151255	4.716769	1.315807
13	1.034318	3.332732	0.540178
7	-2.111278	3.215354	1.342951
6	0.335955	6.010729	1.548547
1	1.390367	6.216969	1.369930
6	-0.479051	7.051507	1.992536
1	-0.063318	8.038593	2.167256
6	-2.363516	5.549011	1.956338
1	-3.422500	5.360200	2.102767
6	-1.833988	6.812720	2.195168
1	-2.489227	7.612247	2.526429
6	1.391183	1.686556	1.534649
6	0.808944	1.520899	2.803301
6	2.074231	0.582754	0.998792
6	0.895275	0.319409	3.502000
6	2.167916	-0.626047	1.687000
6	1.575434	-0.759036	2.940101
1	0.257706	2.348363	3.250310
1	2.525504	0.655056	0.010513
1	0.430432	0.220664	4.478697
1	2.698866	-1.464803	1.246078
1	1.644160	-1.699968	3.477928
6	2.241445	3.997717	-0.856251
6	3.483237	3.403236	-1.136236
6	1.874448	5.104228	-1.642474
6	4.312463	3.878331	-2.150873
6	2.691885	5.585795	-2.662352
6	3.914473	4.969390	-2.918833
1	3.819903	2.555002	-0.542748
1	0.930534	5.613344	-1.446410
1	5.268671	3.399998	-2.341632
1	2.380898	6.442699	-3.252763
1	4.557050	5.341804	-3.710966
6	-3.074021	2.760049	2.287945
6	-4.253364	2.156292	1.844694
6	-2.853204	2.921230	3.658152
6	-5.191440	1.700977	2.764698
6	-3.804408	2.479680	4.571235
6	-4.973306	1.863283	4.130702
1	-4.420686	2.044576	0.777777
1	-1.942216	3.406122	3.994780
1	-6.103006	1.230655	2.410469
1	-3.625377	2.610716	5.633498
1	-5.710470	1.515645	4.846505
6	-1.607839	2.324374	0.392910
6	-1.652171	0.932371	0.600979
6	-0.983388	2.800059	-0.781364
6	-1.076899	0.067274	-0.313879
6	-0.397411	1.905572	-1.690367
6	-0.430170	0.539237	-1.460307
1	-2.096862	0.543456	1.509147
1	-1.037158	3.857138	-1.024410

1	-1.097121	-0.998063	-0.107063
1	0.089773	2.309958	-2.572282
1	0.038469	-0.149520	-2.153528

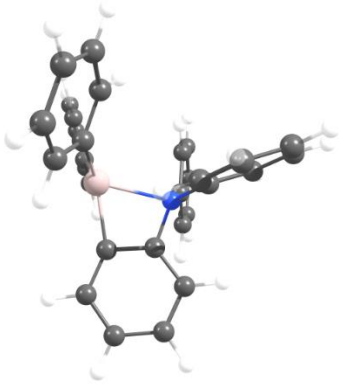

Figure S77: Computed structure of Ph/Ph (CLA)

Data for system: **Ph/Ph (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1454.79965200 A.U.
Zero-point correction= 0.453862 (Hartree/Particle)
Thermal correction to Energy= 0.480530
Thermal correction to Enthalpy= 0.481474
Thermal correction to Gibbs Free Energy= 0.394315

Optimized Geometry (XYZ coordinates in Angstrom)

6	-1.331781	4.974893	1.536396
6	-0.077606	5.508363	1.237920
13	0.705564	3.832779	0.544734
7	-1.473211	3.578566	1.084457
6	0.140944	6.839546	1.611483
1	1.096835	7.315455	1.409326
6	-0.854316	7.568585	2.258902
1	-0.670175	8.599237	2.546638
6	-2.342489	5.662836	2.201709
1	-3.288539	5.180884	2.433407
6	-2.087210	6.982464	2.559707
1	-2.848120	7.557586	3.077541
6	1.728660	2.722004	1.802598
6	2.430757	3.299065	2.874893
6	1.729841	1.318409	1.727503
6	3.100222	2.523250	3.819535
6	2.388797	0.530593	2.668816
6	3.077160	1.134427	3.718043
1	2.444400	4.382675	2.987642
1	1.192941	0.819446	0.921030
1	3.635666	2.999327	4.635846
1	2.364215	-0.552083	2.587073
1	3.592697	0.525162	4.454267
6	0.904324	3.480694	-1.373725

6	1.607944	2.355905	-1.835306
6	0.275284	4.281301	-2.342938
6	1.659570	2.027470	-3.189378
6	0.319740	3.964612	-3.697375
6	1.008120	2.829433	-4.122079
1	2.130479	1.718972	-1.123212
1	-0.282775	5.163032	-2.031517
1	2.207710	1.148707	-3.516782
1	-0.185134	4.597333	-4.421807
1	1.041810	2.575332	-5.177469
6	-1.933351	2.683716	2.140807
6	-3.110177	1.946051	2.022077
6	-1.184561	2.612152	3.317679
6	-3.514303	1.115888	3.066184
6	-1.596097	1.780893	4.350976
6	-2.759977	1.024175	4.229618
1	-3.709138	2.012856	1.121535
1	-0.280316	3.201559	3.419297
1	-4.430538	0.543763	2.962472
1	-0.996824	1.724019	5.253563
1	-3.076553	0.373069	5.037448
6	-2.134464	3.407247	-0.200961
6	-1.960480	2.183510	-0.855975
6	-2.845603	4.430070	-0.816769
6	-2.489562	1.990298	-2.121608
6	-3.369763	4.228844	-2.095782
6	-3.193918	3.018222	-2.751009
1	-1.387571	1.398698	-0.368958
1	-2.969832	5.385604	-0.320939
1	-2.329990	1.045153	-2.629303
1	-3.913986	5.035182	-2.576579
1	-3.593819	2.873210	-3.748835

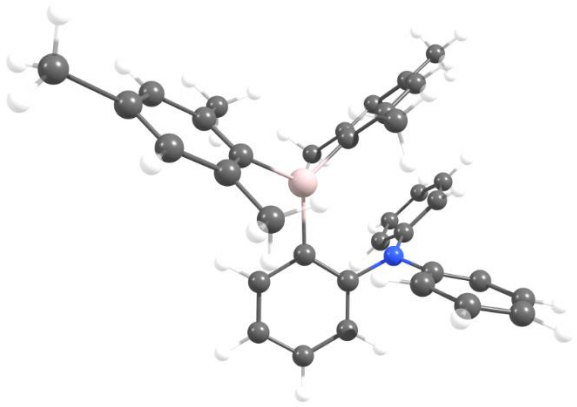

Figure S78: Computed structure of Ph/Mes (FLP)

Data for system: **Ph/Mes (FLP)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1690.65716068 A.U.

Zero-point correction= 0.619590 (Hartree/Particle)
Thermal correction to Energy= 0.656731
Thermal correction to Enthalpy= 0.657675
Thermal correction to Gibbs Free Energy= 0.548072

Optimized Geometry (XYZ coordinates in Angstrom)

6	-1.329794	4.382892	1.441887
6	-0.208792	5.206796	1.619912
13	1.637926	4.605778	1.317968
7	-1.157272	3.046055	0.936164
6	-0.437871	6.491632	2.142775
1	0.411282	7.146295	2.335463
6	-1.717896	6.941805	2.457903
1	-1.863317	7.939530	2.859857
6	-2.616426	4.814167	1.768257
1	-3.453644	4.135733	1.629440
6	-2.809391	6.096320	2.272689
1	-3.810428	6.432154	2.524559
6	2.212604	3.394195	-0.106974
6	2.257915	3.769395	-1.461460
6	1.863392	5.161665	-1.896956
1	2.734168	5.825404	-1.950860
1	1.136023	5.610843	-1.207876
1	1.393496	5.146174	-2.883970
6	2.690560	2.858533	-2.425627
1	2.709556	3.157963	-3.472768
6	3.074324	1.563637	-2.081471
1	2.685214	0.383938	-3.842612
6	3.506518	0.589822	-3.147700
1	4.335973	0.991059	-3.737562
1	3.827180	-0.359872	-2.713756
1	3.302244	0.176758	-0.455857
6	3.017726	1.188566	-0.739018
6	2.594764	2.085212	0.241248
6	2.492334	1.640665	1.683596
1	2.894273	0.635780	1.833637
1	3.046760	2.317206	2.347994
1	1.442548	1.621138	2.012590
6	2.948476	5.362172	2.576742
6	4.049191	6.107933	2.108179
6	4.217101	6.359582	0.626066
1	3.383154	6.953151	0.229341
1	4.249144	5.417899	0.065625
1	5.135575	6.910828	0.411306
6	4.981182	6.634213	3.001765
1	5.821589	7.211727	2.621004
6	4.858748	6.435831	4.376658
1	6.717831	6.267277	5.452782
6	5.893126	6.977246	5.329542
1	6.318932	7.914039	4.961522
1	5.464734	7.159623	6.318071
1	3.658122	5.541069	5.914444
6	3.769984	5.701464	4.843688
6	2.822855	5.169817	3.967706
6	1.657621	4.386266	4.531570
1	1.744938	4.259324	5.613183
1	0.706385	4.890490	4.325749
1	1.600773	3.381747	4.091697
6	-1.588672	1.992730	1.781332

6	-1.253612	2.042317	3.141876
6	-2.359411	0.921023	1.314824
6	-1.664756	1.036309	4.007017
6	-2.755483	-0.086897	2.187984
6	-2.412438	-0.040409	3.536134
1	-0.680022	2.886212	3.513739
1	-2.645069	0.880398	0.269652
1	-1.392508	1.094460	5.056179
1	-3.351675	-0.910344	1.807242
1	-2.727213	-0.828704	4.211186
6	-1.030440	2.868316	-0.461614
6	-0.489444	1.677312	-0.971742
6	-1.386553	3.884683	-1.353171
6	-0.335040	1.506858	-2.337802
6	-1.213293	3.705276	-2.724988
6	-0.695011	2.519355	-3.228822
1	-0.169457	0.900517	-0.284872
1	-1.798616	4.813853	-0.975174
1	0.098486	0.582500	-2.707763
1	-1.496839	4.506900	-3.400581
1	-0.563660	2.384219	-4.297210

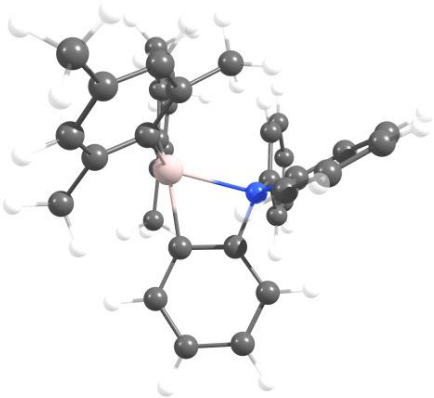

Figure S79: Computed structure of Ph/Mes (CLA)

Data for system: **Ph/Mes (CLA)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1690.65746570 A.U.
Zero-point correction= 0.621216 (Hartree/Particle)
Thermal correction to Energy= 0.657366
Thermal correction to Enthalpy= 0.658310
Thermal correction to Gibbs Free Energy= 0.552820

Optimized Geometry (XYZ coordinates in Angstrom)

6	-1.011851	4.393229	1.558018
6	-0.022700	5.269761	1.992295
13	1.555608	4.244570	1.356759
7	-0.473690	3.262407	0.782377
6	-0.456473	6.389676	2.714601

1	0.264303	7.123396	3.069818
6	-1.806385	6.582569	2.993065
1	-2.124846	7.454556	3.556386
6	-2.369429	4.534005	1.842922
1	-3.089377	3.790458	1.510855
6	-2.761088	5.652712	2.568089
1	-3.809127	5.803195	2.806220
6	2.403518	4.715520	-0.379579
6	1.880810	5.784511	-1.159682
6	0.951387	6.829293	-0.580151
1	1.303649	7.189396	0.390494
1	-0.060457	6.441119	-0.428630
1	0.880524	7.688152	-1.252379
6	2.225304	5.922123	-2.500998
1	1.799035	6.742021	-3.076886
6	3.105500	5.039402	-3.129376
1	2.552431	4.852818	-5.199961
6	3.409814	5.174598	-4.598198
1	3.622157	6.213384	-4.866344
1	4.268810	4.563924	-4.885594
1	4.413092	3.373643	-2.805732
6	3.683698	4.045053	-2.354285
6	3.353088	3.878686	-1.003479
6	4.057079	2.748201	-0.285439
1	5.121312	2.747326	-0.539095
1	3.972588	2.819265	0.799840
1	3.657892	1.774622	-0.594332
6	2.399998	3.178265	2.806005
6	2.848110	3.915519	3.929219
6	2.737369	5.425417	3.962317
1	1.735344	5.738376	4.273890
1	2.932948	5.878917	2.981519
1	3.456361	5.858265	4.662232
6	3.387407	3.273499	5.040661
1	3.731538	3.866418	5.886905
6	3.498471	1.882722	5.093470
1	5.137724	1.478425	6.435560
6	4.085377	1.206570	6.305899
1	3.558697	1.504869	7.217386
1	4.027211	0.119160	6.220413
1	3.165039	0.068207	4.002117
6	3.073156	1.153433	3.990009
6	2.542516	1.778533	2.855845
6	2.165192	0.885061	1.697099
1	3.042632	0.345398	1.324659
1	1.413135	0.144311	1.989097
1	1.754069	1.460041	0.863852
6	-0.853449	1.974169	1.340150
6	-0.749698	1.809082	2.726116
6	-1.294647	0.914003	0.550959
6	-1.056224	0.585812	3.305313
6	-1.596459	-0.311320	1.144278
6	-1.475214	-0.485745	2.517576
1	-0.410782	2.634090	3.343563
1	-1.402168	1.033596	-0.520016
1	-0.955340	0.469808	4.379383
1	-1.935534	-1.130334	0.518196
1	-1.709879	-1.442342	2.971981
6	-0.589996	3.404272	-0.664296
6	0.287983	2.674197	-1.472251

6	-1.481571	4.295323	-1.253851
6	0.281497	2.842745	-2.848576
6	-1.477511	4.466792	-2.639123
6	-0.599978	3.748334	-3.439105
1	0.995002	1.989618	-1.012401
1	-2.156944	4.879608	-0.640570
1	0.988808	2.288109	-3.456110
1	-2.166707	5.176390	-3.085120
1	-0.593289	3.895008	-4.514121

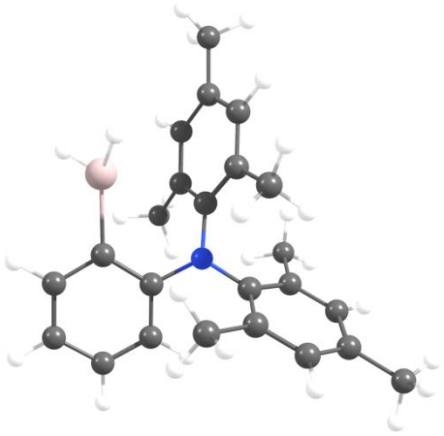

Figure S80: Computed structure of Mes/H

Data for system: **Mes/H**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1228.54660920 A.U.
Zero-point correction= 0.452829 (Hartree/Particle)
Thermal correction to Energy= 0.479192
Thermal correction to Enthalpy= 0.480136
Thermal correction to Gibbs Free Energy= 0.397769

Optimized Geometry (XYZ coordinates in Angstrom)

6	-0.087441	3.410823	0.156441
6	1.282120	3.657393	-0.060009
13	2.402787	2.519379	-1.233373
7	-0.678973	2.206780	-0.329100
6	1.796150	4.853596	0.456962
1	2.846199	5.091724	0.292394
6	1.017346	5.764305	1.169475
1	1.455616	6.675091	1.564085
6	-0.895815	4.333924	0.828844
1	-1.956247	4.135108	0.951967
6	-0.336361	5.498198	1.344563
1	-0.970773	6.204370	1.871639
6	-1.845946	1.675616	0.298146
6	-2.972097	1.366624	-0.484050
6	-1.853219	1.423015	1.686297
6	-4.083683	0.790554	0.134079

6	-2.996277	0.869047	2.256400
1	-4.949788	0.545967	-0.476932
1	-2.995990	0.665976	3.325534
6	-4.122494	0.540302	1.502009
6	-0.079630	1.507034	-1.402608
6	0.136130	0.106074	-1.332551
6	0.305592	2.210701	-2.575518
6	0.737468	-0.534677	-2.409618
6	0.985980	1.514976	-3.591307
1	0.904574	-1.607124	-2.338771
1	1.311197	2.078113	-4.463168
6	1.206976	0.145028	-3.535298
6	-0.071458	3.654081	-2.833431
1	-0.370180	3.759576	-3.879131
1	-0.895932	3.971310	-2.194821
1	0.759900	4.341966	-2.646243
6	-0.187508	-0.705133	-0.105639
1	-1.263409	-0.853019	0.026290
1	0.291007	-1.683569	-0.176378
1	0.185574	-0.207625	0.792817
6	1.945449	-0.581136	-4.627593
1	2.969097	-0.809750	-4.315065
1	1.455659	-1.527430	-4.871483
1	2.000391	0.021363	-5.536644
6	-3.010439	1.636624	-1.966215
1	-2.595157	2.620783	-2.197570
1	-2.429148	0.899871	-2.532050
1	-4.039874	1.603928	-2.328626
6	-5.346006	-0.046241	2.157283
1	-5.991166	-0.536564	1.424858
1	-5.072122	-0.781909	2.918210
1	-5.936016	0.732007	2.652319
6	-0.660078	1.698392	2.565209
1	-0.660873	1.017930	3.419954
1	0.282045	1.583866	2.023261
1	-0.674735	2.725434	2.944182
1	3.216026	3.365879	-2.306152
1	2.937829	1.093703	-0.799022

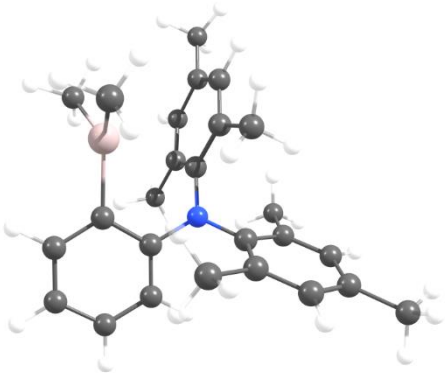

Figure S81: Computed structure of Mes/CH3

Data for system: **Mes/CH3**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1307.19896948 A.U.
Zero-point correction= 0.511529 (Hartree/Particle)
Thermal correction to Energy= 0.541662
Thermal correction to Enthalpy= 0.542606
Thermal correction to Gibbs Free Energy= 0.452648

Optimized Geometry (XYZ coordinates in Angstrom)

6	0.382969	2.889724	0.488394
6	1.736436	2.509329	0.436141
13	2.291685	1.013700	-0.745050
7	-0.544825	2.217285	-0.354869
6	2.620604	3.219697	1.258957
6	2.193297	4.234668	2.115514
1	2.904470	4.755507	2.748466
6	-0.065396	3.912416	1.328180
1	-1.117962	4.182660	1.333781
6	0.843392	4.572634	2.148937
1	0.493919	5.364573	2.804377
6	-1.881125	1.971422	0.074942
6	-2.118998	1.368910	1.329873
6	-2.961589	2.290525	-0.768360
6	-3.433998	1.114374	1.711345
6	-4.257826	1.988590	-0.347378
1	-3.611050	0.643478	2.676287
1	-5.087298	2.232222	-1.007809
6	-4.520914	1.410629	0.890261
6	-0.094950	1.746794	-1.620356
6	-0.310592	0.402591	-2.007583
6	0.484447	2.657171	-2.550852
6	0.064294	-0.000241	-3.295710
6	0.835148	2.197731	-3.813716
1	-0.101476	-1.037177	-3.578095
1	1.279421	2.900793	-4.515062
6	0.638450	0.872884	-4.210790
6	0.727718	4.101428	-2.207016
1	0.793502	4.696735	-3.119955
1	-0.063161	4.505908	-1.571482
1	1.663277	4.217172	-1.647718
6	-0.970998	-0.599253	-1.097748
1	-2.059464	-0.474633	-1.102199
1	-0.735259	-1.613850	-1.425709
1	-0.636936	-0.484507	-0.066001
6	1.068959	0.411670	-5.577684
1	2.160478	0.349785	-5.637226
1	0.663049	-0.574845	-5.810492
1	0.738608	1.110791	-6.350789
6	-1.002243	0.956213	2.254847
1	-0.130238	0.593185	1.703696
1	-0.650621	1.796070	2.863075
1	-1.346778	0.166250	2.925908
6	-5.931382	1.133244	1.341970
1	-5.989848	0.196723	1.902845
1	-6.297408	1.930550	1.997272
1	-6.613413	1.064726	0.491338
6	-2.765142	2.953730	-2.107456
1	-3.712490	3.362400	-2.465103

1	-2.042757	3.770913	-2.039856
1	-2.390930	2.255378	-2.864514
6	3.567952	1.365065	-2.196577
1	4.589949	1.139407	-1.868020
1	3.369258	0.726734	-3.065031
1	3.553944	2.404012	-2.540038
6	2.174656	-0.828403	-0.062493
1	1.497937	-0.966371	0.785802
1	1.876620	-1.533604	-0.846810
1	3.171603	-1.141062	0.273603
1	3.680570	2.969052	1.246341

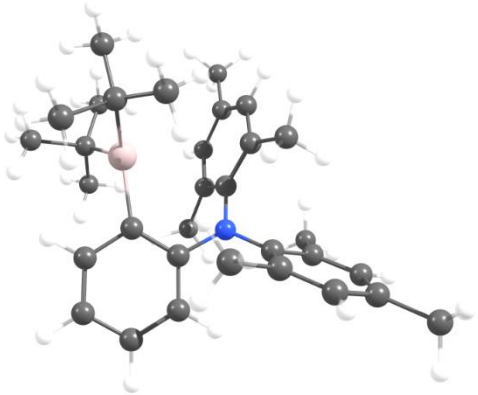

Figure S82: Computed structure of Mes/t-but

Data for system: **Mes/t-but**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1543.01978019 A.U.
Zero-point correction= 0.684315 (Hartree/Particle)
Thermal correction to Energy= 0.721028
Thermal correction to Enthalpy= 0.721972
Thermal correction to Gibbs Free Energy= 0.619477

Optimized Geometry (XYZ coordinates in Angstrom)

6	0.416971	2.781677	0.463510
6	1.780055	2.419670	0.382234
13	2.653294	1.095400	-0.823613
7	-0.568993	2.092931	-0.300783
6	2.664395	3.146538	1.196603
1	3.727819	2.906083	1.170234
6	2.255566	4.170833	2.049490
1	2.977465	4.697013	2.665150
6	-0.003590	3.834547	1.284464
1	-1.053654	4.111398	1.299568
6	0.909529	4.515586	2.081091
1	0.563285	5.325205	2.716244
6	-1.910948	1.990931	0.177861
6	-2.158032	1.504896	1.481439

6	-2.990771	2.325318	-0.660030
6	-3.474265	1.390344	1.918558
6	-4.292917	2.167064	-0.178643
1	-3.655001	1.008584	2.921511
1	-5.121369	2.421663	-0.836018
6	-4.561420	1.714557	1.107819
6	-0.191509	1.505424	-1.533063
6	-0.551612	0.177720	-1.858626
6	0.517889	2.291004	-2.478630
6	-0.085918	-0.365524	-3.058175
6	0.966033	1.687900	-3.656264
1	-0.345186	-1.396704	-3.289130
1	1.510325	2.298049	-4.374279
6	0.704309	0.351117	-3.954968
6	0.718521	3.773802	-2.286328
1	0.868037	4.253910	-3.256233
1	-0.147810	4.224229	-1.796818
1	1.577824	4.004321	-1.652050
6	-1.450594	-0.660335	-0.985318
1	-2.495349	-0.345725	-1.084881
1	-1.379529	-1.710885	-1.275500
1	-1.190990	-0.576055	0.070472
6	1.256958	-0.294095	-5.198038
1	2.200466	-0.806579	-4.979553
1	0.563422	-1.034854	-5.603388
1	1.458870	0.449255	-5.973152
6	-1.050319	1.062070	2.402156
1	-0.214800	0.629396	1.846514
1	-0.638865	1.901311	2.972435
1	-1.426355	0.318020	3.107932
6	-5.972875	1.588924	1.619522
1	-6.106354	0.663634	2.186593
1	-6.223508	2.419989	2.286849
1	-6.693516	1.592776	0.798679
6	-2.802026	2.833057	-2.066459
1	-3.733874	3.267153	-2.434415
1	-2.027319	3.600420	-2.114608
1	-2.506346	2.034173	-2.755861
6	4.167101	1.767816	-1.971019
6	2.815820	-0.785783	-0.153094
6	4.077106	3.254358	-2.330810
1	3.912631	3.887948	-1.450817
1	5.013315	3.586237	-2.806038
1	3.269221	3.450109	-3.042979
6	5.440250	1.580487	-1.118026
1	5.633849	0.530768	-0.873830
1	6.316676	1.947106	-1.674489
1	5.407189	2.143185	-0.176514
6	4.363865	0.975828	-3.271757
1	5.280468	1.310904	-3.782174
1	4.463672	-0.100421	-3.099535
1	3.533169	1.125182	-3.968917
6	1.504101	-1.485299	0.198616
1	0.941180	-1.761227	-0.697694
1	1.705746	-2.410898	0.760522
1	0.859447	-0.859640	0.825229
6	3.620364	-1.723831	-1.059407
1	4.626276	-1.347121	-1.270476
1	3.739553	-2.707092	-0.578049
1	3.117176	-1.888516	-2.019974

6	3.591840	-0.578759	1.166701
1	3.779178	-1.551160	1.647713
1	4.569889	-0.103909	1.020731
1	3.025470	0.033163	1.879382

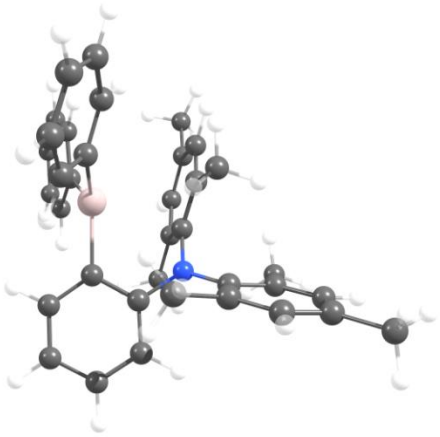

Figure S83: Computed structure of Mes/Ph

Data for system: **Mes/Ph**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1690.66852574 A.U.
Zero-point correction= 0.621616 (Hartree/Particle)
Thermal correction to Energy= 0.657836
Thermal correction to Enthalpy= 0.658780
Thermal correction to Gibbs Free Energy= 0.552124

Optimized Geometry (XYZ coordinates in Angstrom)

6	0.385559	3.316451	0.018708
6	1.730463	2.906770	-0.067889
13	2.124908	1.007338	-0.445972
7	-0.634319	2.358864	-0.237588
6	2.706661	3.887576	0.152266
1	3.759593	3.617017	0.084925
6	2.379146	5.205839	0.471452
1	3.159644	5.939196	0.645936
6	0.037169	4.633703	0.326554
1	-1.011193	4.914826	0.378554
6	1.038654	5.570022	0.563309
1	0.766261	6.592911	0.805009
6	-1.869566	2.384168	0.474441
6	-1.869027	2.475186	1.884087
6	-3.088201	2.272637	-0.221547
6	-3.089528	2.480767	2.555165
6	-4.280348	2.253908	0.504448
1	-3.081651	2.545840	3.641292
1	-5.217029	2.161276	-0.041021
6	-4.309196	2.369780	1.890177
6	-0.354940	1.332544	-1.183793

6	-0.516825	-0.032592	-0.844028
6	0.001011	1.687064	-2.518120
6	-0.278028	-1.003802	-1.829316
6	0.219088	0.679976	-3.447116
1	-0.398286	-2.049679	-1.555890
1	0.514149	0.959183	-4.456123
6	0.098609	-0.675041	-3.124863
6	0.149251	3.123352	-2.940428
1	0.073963	3.203906	-4.026487
1	-0.609180	3.759991	-2.478632
1	1.117702	3.528901	-2.628610
6	-1.014628	-0.471392	0.508481
1	-2.098086	-0.325468	0.582459
1	-0.788362	-1.527720	0.665579
1	-0.548627	0.093711	1.317225
6	0.410459	-1.730977	-4.149756
1	0.088854	-2.719318	-3.814571
1	-0.080290	-1.512578	-5.102228
1	1.489985	-1.764041	-4.331329
6	-0.598186	2.515986	2.693278
1	-0.168527	3.522471	2.728618
1	-0.798632	2.191133	3.716647
1	0.171327	1.863653	2.271071
6	-5.611053	2.393072	2.648308
1	-5.522530	1.865392	3.601563
1	-5.917514	3.420703	2.870088
1	-6.413184	1.925556	2.072543
6	-3.154076	2.171302	-1.723973
1	-4.175436	2.350886	-2.065768
1	-2.500929	2.905834	-2.200271
1	-2.846114	1.183998	-2.086253
6	3.141264	0.554701	-2.060370
6	3.531584	-0.760700	-2.360576
6	3.481537	1.547778	-2.995181
6	4.202279	-1.076771	-3.541756
6	4.152555	1.246578	-4.177883
6	4.506841	-0.071848	-4.456797
1	3.313703	-1.561270	-1.655873
1	3.215228	2.585108	-2.795243
1	4.489909	-2.104088	-3.747128
1	4.401285	2.036111	-4.881056
1	5.028228	-0.313290	-5.378230
6	2.201822	-0.201751	1.101824
6	2.453814	0.337578	2.374781
6	2.053947	-1.597593	1.023517
6	2.549319	-0.466649	3.510584
6	2.144551	-2.411678	2.149080
6	2.392970	-1.844486	3.398031
1	2.571309	1.415479	2.486563
1	1.839267	-2.063611	0.061695
1	2.742535	-0.018447	4.480754
1	2.020933	-3.486818	2.056417
1	2.462664	-2.475615	4.278781

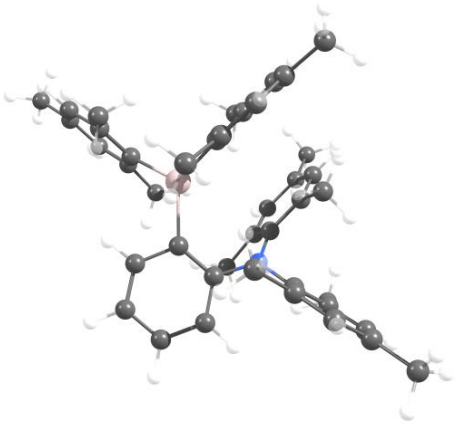

Figure S84: Computed structure of Mes/Mes

Data for system: **Mes/Mes**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1926.52407156 A.U.
Zero-point correction= 0.788584 (Hartree/Particle)
Thermal correction to Energy= 0.834684
Thermal correction to Enthalpy= 0.835628
Thermal correction to Gibbs Free Energy= 0.708546

Optimized Geometry (XYZ coordinates in Angstrom)

6	-0.398363	3.527422	0.535230
6	0.908916	3.599496	1.066119
13	2.082298	2.209781	1.797374
7	-1.014772	2.282540	0.242111
6	1.452817	4.884710	1.252386
1	2.474992	4.972756	1.622773
6	0.740355	6.053399	0.992954
1	1.192017	7.025022	1.162797
6	-1.119256	4.698794	0.267987
1	-2.120162	4.621406	-0.146093
6	-0.559148	5.947795	0.508984
1	-1.137658	6.840525	0.291115
6	-2.436666	2.173544	0.362445
6	-3.235169	1.779388	-0.726318
6	-3.033894	2.435471	1.613765
6	-4.612054	1.639827	-0.531624
6	-4.412371	2.304833	1.747940
1	-5.223393	1.328331	-1.375841
1	-4.861465	2.500499	2.719645
6	-5.224860	1.902802	0.688413
6	-0.289612	1.215408	-0.363258
6	-0.514288	-0.109663	0.070720
6	0.553101	1.457549	-1.475316
6	0.094531	-1.156614	-0.622793
6	1.170159	0.371738	-2.099617
1	-0.087021	-2.173474	-0.279737
1	1.814847	0.566826	-2.954518

6	0.949067	-0.944843	-1.700776
6	1.480315	0.674123	2.861701
6	0.739084	0.770742	4.051834
6	1.823712	-0.611766	2.390351
6	0.279666	-0.387026	4.690292
6	1.362748	-1.750195	3.044228
1	-0.310199	-0.296383	5.600903
1	1.623419	-2.734826	2.658776
6	0.564842	-1.653211	4.188538
6	4.021000	2.580211	1.747062
6	4.738858	2.692493	2.958046
6	4.743130	2.696532	0.543779
6	6.118415	2.893320	2.949980
6	6.125928	2.889789	0.558820
1	6.651464	2.981445	3.895008
1	6.663832	2.973426	-0.383856
6	6.832231	2.984751	1.755219
6	4.018124	2.614280	4.286021
1	3.550933	1.633729	4.430533
1	4.699196	2.792202	5.121589
1	3.223506	3.369068	4.350003
6	8.329018	3.159554	1.762875
1	8.649507	3.791907	2.594847
1	8.833532	2.193667	1.872151
1	8.680230	3.612358	0.832613
6	0.735357	2.827846	-2.079073
1	1.177844	2.738314	-3.073610
1	-0.218698	3.354364	-2.168859
1	1.377123	3.470432	-1.471223
6	-1.395027	-0.442506	1.246850
1	-2.457933	-0.386201	0.989484
1	-1.173799	-1.453313	1.596426
1	-1.215220	0.242534	2.078884
6	1.648875	-2.092117	-2.380423
1	2.625111	-2.280646	-1.919261
1	1.065249	-3.012766	-2.305592
1	1.822517	-1.881031	-3.438633
6	-2.671930	1.506371	-2.097542
1	-1.959430	2.278831	-2.394847
1	-2.144692	0.547482	-2.142951
1	-3.478798	1.487082	-2.833189
6	-6.716520	1.778503	0.861473
1	-7.161922	1.196937	0.051192
1	-6.964837	1.290375	1.807900
1	-7.194819	2.763457	0.866820
6	2.739260	-0.746866	1.194378
1	3.771708	-0.500013	1.467024
1	2.724508	-1.760173	0.783931
1	2.438934	-0.076042	0.376865
6	0.487806	2.106778	4.714647
1	1.236939	2.289964	5.493573
1	0.540842	2.940511	4.003830
1	-0.495721	2.144697	5.191581
6	0.019523	-2.893604	4.848085
1	-0.859487	-3.264475	4.309811
1	0.760952	-3.697001	4.855696
1	-0.282664	-2.695645	5.879011
6	-2.202848	2.806186	2.810368
1	-2.754799	2.612116	3.733207
1	-1.277487	2.224609	2.824263

1	-1.912706	3.862830	2.796919
6	4.029527	2.666840	-0.787202
1	4.720223	2.471552	-1.611559
1	3.249216	1.896308	-0.824776
1	3.545106	3.630913	-0.980131

4.2. Dimers

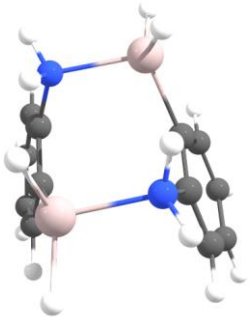

Figure S85: Computed structure of H/H.

Data for system: **H/H**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1061.28894020 A.U.
Zero-point correction= 0.250197 (Hartree/Particle)
Thermal correction to Energy= 0.265660
Thermal correction to Enthalpy= 0.266604
Thermal correction to Gibbs Free Energy= 0.208002

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.560852	4.826209	2.273043
6	1.213708	5.130209	2.044254
13	-0.193400	4.988090	3.444563
7	2.939640	4.331349	3.594546
6	0.899611	5.528384	0.736566
1	-0.131651	5.779180	0.497433
6	1.858821	5.607796	-0.272619
1	1.573930	5.916592	-1.273249
6	3.541946	4.887433	1.290907
1	4.571645	4.623409	1.520555
6	3.182233	5.284601	0.005545
1	3.937740	5.339063	-0.771409
1	3.916066	4.548847	3.792940
1	0.383525	5.381066	4.894999
1	-1.645314	5.447075	2.992743
1	2.372810	4.797411	4.310194
6	-0.631482	1.214388	0.456343
6	0.695019	0.837986	0.277652
1	0.992739	0.308061	-0.621420
1	-1.376588	0.981751	-0.297386
6	-1.007780	1.895897	1.611033

6	1.640748	1.148618	1.254360
1	2.674740	0.851365	1.092976
6	1.309795	1.836284	2.431120
6	-0.039824	2.182790	2.565786
1	-2.039930	2.204507	1.759781
7	-0.434936	2.968784	3.732359
13	2.698597	2.299883	3.779181
1	4.155599	1.750317	3.465694
1	2.101888	2.252804	5.273348
1	0.122020	2.681565	4.543516
1	-1.414125	2.801549	3.963152

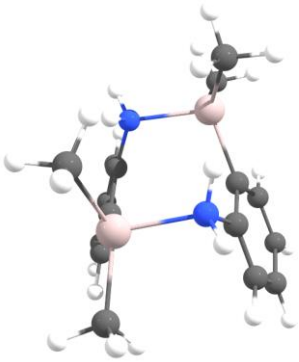

Figure S86: Computed structure of H/CH_3.

Data for system: **H/CH_3**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1218.58429479 A.U.
Zero-point correction= 0.365521 (Hartree/Particle)
Thermal correction to Energy= 0.389846
Thermal correction to Enthalpy= 0.390790
Thermal correction to Gibbs Free Energy= 0.311811

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.515625	4.774441	1.618931
6	1.175276	5.077559	1.354781
13	-0.337240	4.929558	2.657063
7	2.859102	4.260287	2.941046
6	0.907552	5.504873	0.044982
1	-0.116011	5.757316	-0.225832
6	1.899003	5.613191	-0.930276
1	1.645815	5.945416	-1.932029
6	3.529388	4.862405	0.671832
1	4.552117	4.599550	0.932706
6	3.213518	5.288451	-0.615754
1	3.995238	5.364619	-1.364522
1	3.821892	4.500591	3.177962
1	2.260916	4.700450	3.643656
6	-0.646081	1.036313	-0.200569
6	0.681312	0.652974	-0.353333
1	0.987077	0.089259	-1.228960

1	-1.385681	0.776102	-0.950781
6	-1.029594	1.759824	0.925792
6	1.618018	1.000731	0.620076
1	2.653060	0.696485	0.475734
6	1.281454	1.731384	1.770153
6	-0.069231	2.080913	1.878180
1	-2.063180	2.071830	1.057934
7	-0.481439	2.897768	3.015317
13	2.722370	2.201084	3.077489
1	0.073048	2.643892	3.835863
1	-1.457841	2.716507	3.249098
6	-2.096109	5.323588	1.856041
1	-2.264608	4.768669	0.925153
1	-2.927808	5.082649	2.529584
1	-2.203122	6.385547	1.607134
6	0.048231	5.594897	4.494445
1	-0.870375	5.589428	5.094292
1	0.784134	5.033772	5.087712
1	0.390507	6.636399	4.479616
6	4.518609	1.639302	2.487460
1	5.315940	2.044083	3.122942
1	4.634915	0.549750	2.508823
1	4.735416	1.954148	1.459430
6	2.234871	1.997371	4.997759
1	1.468749	2.677908	5.395637
1	1.890805	0.979880	5.217759
1	3.118701	2.158178	5.627577

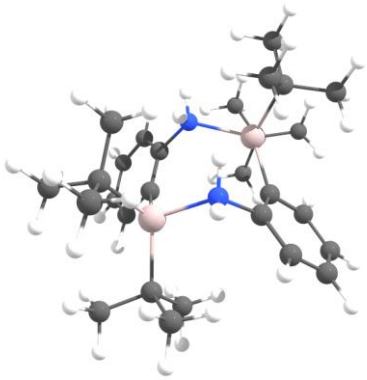

Figure S87: Computed structure of H/*t*-but.

Data for system: **H/*t*-but**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1690.23081218 A.U.
Zero-point correction= 0.710413 (Hartree/Particle)
Thermal correction to Energy= 0.749566
Thermal correction to Enthalpy= 0.750510
Thermal correction to Gibbs Free Energy= 0.643192

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.926529	4.873151	1.806728

6	1.716397	5.101529	1.138803
13	-0.178078	4.843545	1.768642
7	2.959640	3.917925	2.916089
6	1.819855	5.946314	0.017382
1	0.924947	6.166186	-0.559061
6	3.014377	6.533837	-0.396217
1	3.033093	7.169445	-1.275545
6	4.123701	5.492386	1.456584
1	5.018527	5.336190	2.052255
6	4.171380	6.323064	0.341927
1	5.105213	6.799483	0.063127
1	3.836157	4.021210	3.432788
1	2.223003	4.148323	3.586425
6	-1.190821	-0.007384	0.757154
6	0.068135	-0.382876	0.307689
1	0.181977	-1.232663	-0.357471
1	-2.075765	-0.562782	0.465346
6	-1.310888	1.094244	1.597717
6	1.190019	0.322018	0.740910
1	2.163388	-0.024609	0.403377
6	1.124149	1.440476	1.593345
6	-0.175113	1.812505	1.962862
1	-2.288838	1.384549	1.970854
7	-0.371326	3.030351	2.751938
13	2.890870	1.902411	2.440558
1	0.237980	3.006480	3.572373
1	-1.323696	3.049001	3.124206
6	-0.461337	6.084811	3.336567
6	-1.572819	4.814900	0.323995
6	4.508683	1.571401	1.297928
6	2.875998	1.139486	4.310630
6	-1.889417	6.012244	3.891162
1	-2.631325	6.301188	3.138562
1	-2.156948	5.006617	4.247284
1	-2.017334	6.691443	4.749145
6	-0.194397	7.525665	2.873038
1	0.824920	7.643734	2.485592
1	-0.884964	7.838097	2.082102
1	-0.314221	8.236091	3.706658
6	0.514574	5.797093	4.485383
1	0.420156	4.776880	4.891080
1	1.556376	5.960931	4.176254
1	0.339487	6.473836	5.336543
6	-1.913992	6.246390	-0.126675
1	-1.047235	6.814268	-0.482803
1	-2.642415	6.220243	-0.952399
1	-2.370594	6.826082	0.684553
6	-1.103225	4.005570	-0.895268
1	-0.191291	4.414739	-1.342952
1	-0.894815	2.960303	-0.636163
1	-1.878797	4.002078	-1.677727
6	-2.890773	4.196083	0.817329
1	-3.669592	4.289527	0.044263
1	-2.788334	3.127117	1.021375
1	-3.278034	4.684121	1.719859
6	4.887503	0.079661	1.313754
1	5.192986	-0.248314	2.314658
1	4.078479	-0.583684	0.988065
1	5.741548	-0.101340	0.642206
6	5.739406	2.331414	1.818662

1	5.958238	2.116453	2.871541
1	6.634530	2.049775	1.242207
1	5.628944	3.412896	1.704198
6	4.269299	2.010550	-0.155488
1	5.164579	1.819197	-0.768346
1	3.435187	1.476045	-0.622358
1	4.046774	3.082256	-0.226993
6	2.656649	-0.378707	4.216083
1	2.619130	-0.834391	5.218556
1	1.713799	-0.620440	3.710444
1	3.461955	-0.877310	3.665767
6	4.191911	1.392454	5.056784
1	4.157993	0.973457	6.075169
1	5.042847	0.928428	4.546033
1	4.419176	2.462854	5.167904
6	1.727975	1.704677	5.157497
1	0.749571	1.439563	4.733105
1	1.741045	1.287314	6.176684
1	1.776972	2.798445	5.282512

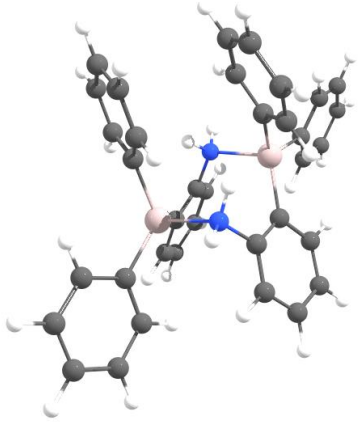

Figure S88: Computed structure of H/Ph.

Data for system: **H/Ph**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1985.52708228 A.U.
Zero-point correction= 0.587289 (Hartree/Particle)
Thermal correction to Energy= 0.622956
Thermal correction to Enthalpy= 0.623901
Thermal correction to Gibbs Free Energy= 0.516455

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.492298	4.802572	0.556364
6	1.121551	4.934905	0.296741
13	-0.333903	4.553053	1.601266
7	2.915176	4.302880	1.860725
6	0.795560	5.400875	-0.987327
1	-0.252291	5.545837	-1.242298
6	1.761619	5.688902	-1.951079

1	1.463836	6.042611	-2.932892
6	3.481160	5.078226	-0.382365
1	4.530548	4.942424	-0.130493
6	3.107836	5.520841	-1.648754
1	3.871252	5.739545	-2.388302
1	3.863221	4.622539	2.063752
1	2.310269	4.681870	2.598379
6	-0.240200	0.416543	-1.055922
6	1.121381	0.183321	-1.209787
1	1.480482	-0.421428	-2.036278
1	-0.954591	-0.000707	-1.758150
6	-0.692772	1.183245	0.014782
6	2.023807	0.730010	-0.297728
1	3.084787	0.529780	-0.432860
6	1.617558	1.524726	0.786633
6	0.233954	1.711128	0.907828
1	-1.755175	1.373855	0.149229
7	-0.270028	2.542313	1.996358
13	2.987047	2.260304	2.031579
1	0.281529	2.383657	2.847364
1	-1.232137	2.280686	2.215659
6	0.078646	5.233589	3.422867
6	0.891162	6.366841	3.617185
6	-0.390833	4.598502	4.587148
6	1.221711	6.836000	4.888942
6	-0.079381	5.060407	5.863221
6	0.732894	6.181812	6.016070
1	1.280195	6.900200	2.748324
1	-1.018802	3.709575	4.509226
1	1.852472	7.713309	5.000113
1	-0.455226	4.537624	6.737855
1	0.984382	6.542315	7.008991
6	-2.176744	4.748996	0.928066
6	-2.598915	4.243342	-0.316492
6	-3.158403	5.367929	1.721790
6	-3.920891	4.346837	-0.745083
6	-4.483997	5.479648	1.303702
6	-4.867150	4.967471	0.067420
1	-1.878219	3.755924	-0.973064
1	-2.880648	5.777450	2.692249
1	-4.213343	3.948353	-1.712352
1	-5.216843	5.966741	1.940395
1	-5.897951	5.052783	-0.263159
6	2.449566	2.098410	3.938476
6	1.605157	1.062127	4.380264
6	2.855745	3.027439	4.913843
6	1.184115	0.959795	5.706589
6	2.453935	2.933108	6.243666
6	1.611513	1.897599	6.642106
1	1.263317	0.310916	3.666341
1	3.504955	3.859974	4.638203
1	0.530675	0.147105	6.010627
1	2.782713	3.675067	6.965447
1	1.289278	1.823412	7.676415
6	4.867555	1.908507	1.554863
6	5.795373	1.538619	2.544324
6	5.367924	2.063692	0.247810
6	7.143479	1.333366	2.252882
6	6.713094	1.863520	-0.056160
6	7.604456	1.496650	0.949634

1	5.456443	1.403480	3.570733
1	4.691233	2.347110	-0.558316
1	7.833459	1.044984	3.040581
1	7.066367	1.989103	-1.075653
1	8.653123	1.337035	0.717460

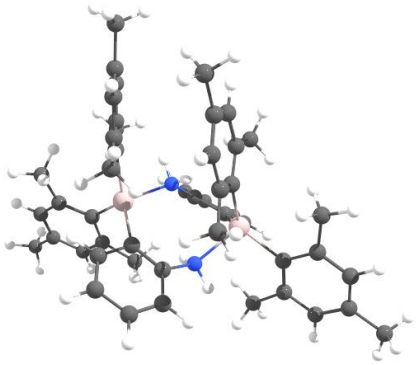

Figure S89: Computed structure of H/Mes.

Data for system: **H/Mes**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -2457.22299896 A.U.
Zero-point correction= 0.922288 (Hartree/Particle)
Thermal correction to Energy= 0.976917
Thermal correction to Enthalpy= 0.977861
Thermal correction to Gibbs Free Energy= 0.833559

Optimized Geometry (XYZ coordinates in Angstrom)

6	1.918572	6.780764	3.602782
6	0.666531	7.104158	3.072507
13	-0.872675	6.005274	2.379695
7	2.306857	5.382533	3.760911
6	0.360559	8.479954	3.091357
1	-0.617454	8.806612	2.736711
6	1.242452	9.457891	3.538362
1	0.953716	10.503749	3.520511
6	2.824464	7.735269	4.067648
1	3.789402	7.421715	4.461679
6	2.494426	9.082384	4.018217
1	3.200185	9.826948	4.371232
1	3.039957	5.344010	4.469935
1	1.513834	4.888525	4.179378
6	-0.542706	0.999980	4.042628
6	0.790504	0.667350	4.269304
1	1.039483	-0.225388	4.834187
1	-1.340263	0.376582	4.433429
6	-0.853719	2.136544	3.304105
6	1.801718	1.487935	3.772942
1	2.838993	1.217695	3.968801
6	1.538496	2.653016	3.032687
6	0.182007	2.927932	2.810539

1	-1.888864	2.415405	3.118103
7	-0.189363	4.077070	1.993166
13	2.983495	3.914711	2.417011
1	-0.934987	3.783850	1.360804
1	0.583792	4.302825	1.352834
1	-3.094292	7.965791	1.841536
1	-4.803735	7.943529	2.287936
6	-3.908252	7.324418	2.192581
1	-4.090798	6.596805	1.395904
6	-3.578873	6.660115	3.513252
6	-2.320087	6.060848	3.757990
6	-4.565272	6.682796	4.502524
1	-5.523451	7.151695	4.285010
6	-4.353586	6.133100	5.763721
6	-3.100157	5.589702	6.031741
1	-2.895631	5.191554	7.024111
6	-2.096371	5.561873	5.062237
6	-0.736529	5.044877	5.481138
1	-0.009376	5.866501	5.495564
1	-0.372613	4.259910	4.808841
1	-0.766816	4.611340	6.483738
1	-6.058322	5.223054	6.719466
6	-5.444377	6.126246	6.803273
1	-5.029220	6.148627	7.814025
1	-6.108548	6.986255	6.686065
1	-4.158311	4.253191	0.503956
6	-3.102848	4.244699	0.791745
1	-3.063254	4.498548	1.855104
1	-2.771335	3.202883	0.670394
6	-2.312287	5.201491	-0.091276
6	-2.581480	5.110798	-1.459269
1	-3.309094	4.378853	-1.809122
6	-1.950066	5.936777	-2.382191
6	-2.223349	5.807113	-3.858624
1	-1.778413	4.890397	-4.261156
1	-3.297105	5.761801	-4.061956
1	-1.806921	6.651577	-4.413434
6	-1.055545	6.881176	-1.888965
1	-0.567926	7.559563	-2.587013
1	-0.315036	8.879661	0.418150
6	0.200530	8.078494	-0.122631
1	0.993533	7.702549	0.526412
1	0.671902	8.524021	-1.003108
6	-0.762454	6.987203	-0.527463
6	-1.372867	6.133033	0.422156
1	0.767048	2.119140	0.317379
6	1.743570	2.256403	-0.161078
1	2.480282	1.785420	0.496351
1	1.725116	1.693334	-1.097313
6	2.069467	3.712694	-0.434021
6	1.774806	4.200544	-1.706003
1	1.290734	3.545192	-2.428432
6	2.106719	5.500533	-2.088063
6	1.808808	5.992356	-3.480122
1	2.531607	5.591831	-4.198917
1	0.811220	5.677577	-3.799610
1	1.855614	7.083344	-3.531948
6	2.775109	6.294760	-1.164983
1	3.084763	7.299097	-1.451791
1	3.245919	7.636585	1.331362

6	3.844281	6.773024	1.020828
1	4.207718	6.276569	1.927458
1	4.722423	7.156352	0.491125
6	3.061648	5.838028	0.125647
6	2.681905	4.544907	0.542586
6	5.735907	3.456792	0.731593
1	4.931251	2.829094	0.336223
1	6.657999	3.181777	0.214099
1	5.489766	4.486826	0.455483
6	5.896485	3.299994	2.228538
6	7.164389	2.974136	2.703060
6	7.418670	2.797611	4.063635
6	8.800517	2.442845	4.547724
1	7.979998	2.846301	1.993393
1	9.148610	1.510956	4.091996
1	9.520962	3.222650	4.282257
1	8.821529	2.318109	5.632649
6	6.356006	2.950190	4.942137
1	6.523641	2.805012	6.008216
1	4.192859	2.711600	6.381791
6	4.020011	3.432022	5.577749
1	3.002193	3.263178	5.218631
1	4.066343	4.424516	6.047999
6	5.071281	3.280736	4.492994
6	4.802214	3.472701	3.119066

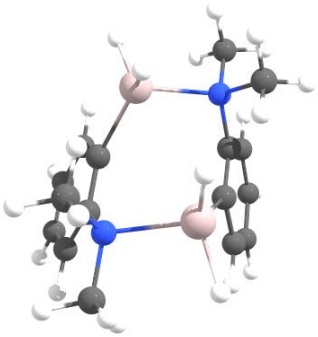

Figure S90: Computed structure of CH_3/H.

Data for system: **CH_3/H**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1218.46406534 A.U.
Zero-point correction= 0.365463 (Hartree/Particle)
Thermal correction to Energy= 0.385588
Thermal correction to Enthalpy= 0.386532
Thermal correction to Gibbs Free Energy= 0.319048

Optimized Geometry (XYZ coordinates in Angstrom)

6	3.060384	4.339146	2.137399
6	1.819738	4.987162	1.970004
13	0.352136	4.877178	0.602837
7	3.526379	3.404105	1.089828

6	1.450650	5.868922	2.999149
1	0.509821	6.408046	2.907739
6	2.226143	6.090967	4.136998
1	1.887699	6.777207	4.906713
6	3.852316	4.551084	3.264751
1	4.802943	4.051593	3.394380
6	3.431029	5.423277	4.267847
1	4.058602	5.572826	5.140511
1	-0.568092	6.167006	0.787659
1	0.655896	4.424684	-0.890516
6	-0.673635	1.959609	4.700427
6	0.525600	1.273773	4.621741
1	0.912633	0.736156	5.481450
1	-1.248311	1.972820	5.620930
6	-1.158037	2.638732	3.583048
6	1.231744	1.283203	3.419036
1	2.168767	0.731925	3.371269
6	0.797927	1.966761	2.271271
6	-0.434435	2.640631	2.391684
1	-2.102386	3.157944	3.675876
7	-0.965261	3.375600	1.222453
13	2.182864	1.823003	0.823641
1	1.791638	2.004896	-0.706431
1	3.118686	0.581394	1.180373
6	3.718543	4.130111	-0.198598
1	4.460803	4.923049	-0.057877
1	4.066921	3.417937	-0.948876
1	2.777500	4.552171	-0.540551
6	4.821366	2.756034	1.408487
1	4.739829	2.186299	2.333976
1	5.061388	2.061380	0.603526
1	5.614763	3.506684	1.492005
6	-1.227512	2.432559	0.097315
1	-0.305184	1.954065	-0.220081
1	-1.953920	1.679338	0.420554
1	-1.625228	3.001013	-0.745395
6	-2.243453	4.076353	1.494249
1	-2.533140	4.617125	0.593242
1	-3.026522	3.356428	1.755833
1	-2.112202	4.802001	2.296653

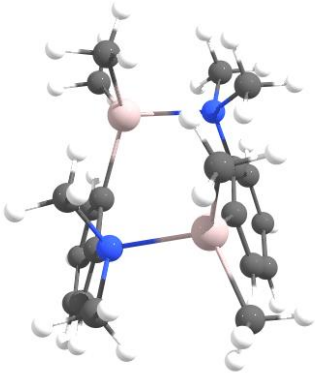

Figure S91: Computed structure of CH_3/CH_3.

Data for system: **CH_3/CH_3**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1375.74794959 A.U.
Zero-point correction= 0.483054 (Hartree/Particle)
Thermal correction to Energy= 0.510508
Thermal correction to Enthalpy= 0.511452
Thermal correction to Gibbs Free Energy= 0.429892

Optimized Geometry (XYZ coordinates in Angstrom)

6	3.104448	4.336772	2.115004
6	1.853356	4.994165	2.044579
13	0.272120	5.071376	0.754407
7	3.524259	3.447454	1.011685
6	1.544858	5.782518	3.168148
1	0.604136	6.323304	3.184273
6	2.368601	5.913902	4.286068
1	2.058142	6.531923	5.122529
6	3.947938	4.463804	3.218658
1	4.904462	3.961460	3.259905
6	3.579136	5.247928	4.309719
1	4.248110	5.328653	5.160387
6	-0.806506	2.248765	4.723837
6	0.402878	1.581273	4.757518
1	0.762511	1.129326	5.676435
1	-1.425485	2.334651	5.611059
6	-1.239968	2.815521	3.527066
6	1.161339	1.494024	3.590044
1	2.103255	0.958966	3.654721
6	0.786703	2.059196	2.357459
6	-0.461421	2.726030	2.373224
1	-2.194805	3.322738	3.527147
7	-0.948212	3.392307	1.147003
13	2.292431	1.730385	1.017175
6	3.505907	4.180224	-0.282157
1	4.206130	5.021204	-0.227308
1	3.805097	3.497200	-1.078171
1	2.513080	4.552628	-0.499323
6	4.904414	2.923808	1.150492
1	5.005840	2.322677	2.050450
1	5.106359	2.283079	0.290418
1	5.623793	3.750282	1.164423
6	-1.000260	2.426575	0.017383
1	-0.019683	2.012997	-0.180109
1	-1.692674	1.616147	0.271009
1	-1.346816	2.947530	-0.876014
6	-2.320695	3.941269	1.262219
1	-2.574400	4.408364	0.309073
1	-3.034148	3.136866	1.473659
1	-2.373732	4.702784	2.036136
6	2.066064	1.408287	-0.932659
1	3.057281	1.166406	-1.340982
1	1.456410	0.510189	-1.098014
1	1.649542	2.197000	-1.566027
6	3.447415	0.274931	1.726607
1	3.958912	0.433868	2.682737

1	2.824740	-0.619426	1.862262
1	4.219142	-0.000775	0.997546
6	0.384606	5.016195	-1.230813
1	0.979861	5.862552	-1.598002
1	0.767458	4.118849	-1.725726
1	-0.629291	5.183021	-1.620712
6	-0.845884	6.643128	1.239498
1	-0.218947	7.542082	1.170272
1	-1.657762	6.782784	0.515179
1	-1.303366	6.670721	2.235041

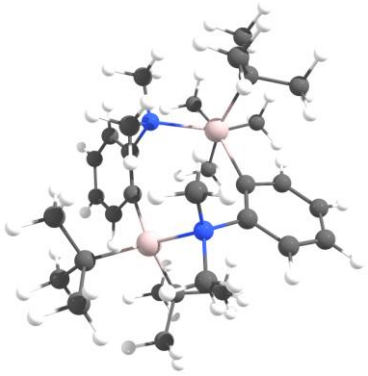

Figure S92: Computed structure of CH_3/*t*-but.

Data for system: **CH_3/*t*-but**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1847.36050163 A.U.
Zero-point correction= 0.830963 (Hartree/Particle)
Thermal correction to Energy= 0.872950
Thermal correction to Enthalpy= 0.873894
Thermal correction to Gibbs Free Energy= 0.763209

Optimized Geometry (XYZ coordinates in Angstrom)

6	0.224853	2.294982	0.001624
6	1.219152	1.391635	0.441542
13	2.050098	-0.450790	-0.009382
7	-0.804300	1.840021	-0.961706
6	-1.248338	-1.438024	0.325801
6	-0.353008	-2.383576	-0.209946
7	0.779685	-1.938979	-1.058854
13	-2.066174	0.428477	0.042922
6	3.575255	0.077187	-1.314869
6	2.700298	-1.536708	1.643292
6	-2.551483	1.296051	1.856847
6	-3.675122	0.172953	-1.216403
6	4.351131	-1.034021	-2.043033
1	4.674523	-1.843945	-1.379868
1	3.774092	-1.473566	-2.866297
1	5.258709	-0.614264	-2.503212
6	4.606425	0.810755	-0.425783
1	4.217749	1.760816	-0.049255

1	4.940193	0.218893	0.433670
1	5.502698	1.048140	-1.019150
6	3.174411	1.098752	-2.391006
1	2.520750	0.669243	-3.161866
1	2.667549	1.969312	-1.959383
1	4.070852	1.469248	-2.912512
6	3.104457	-0.648088	2.839339
1	2.277885	-0.028358	3.201895
1	3.416901	-1.294763	3.672733
1	3.958733	0.003008	2.620247
6	1.651418	-2.502821	2.228471
1	0.693359	-2.013980	2.439778
1	1.439332	-3.357355	1.583131
1	2.027795	-2.918596	3.175517
6	3.963607	-2.366925	1.329795
1	4.271349	-2.921846	2.229559
1	3.829068	-3.109366	0.537424
1	4.812011	-1.739756	1.038196
6	-3.828499	0.698906	2.499240
1	-4.683418	0.663237	1.815571
1	-3.687379	-0.303147	2.912497
1	-4.128261	1.326391	3.351783
6	-2.854097	2.804975	1.780686
1	-3.693253	3.031186	1.110099
1	-3.140094	3.173702	2.777506
1	-1.988429	3.395324	1.476579
6	-1.408275	1.110005	2.871094
1	-1.716726	1.471739	3.864730
1	-1.124156	0.055860	2.979863
1	-0.508720	1.666639	2.586278
6	-4.413234	-1.105723	-0.768604
1	-5.321251	-1.241380	-1.376908
1	-3.799120	-2.003854	-0.888813
1	-4.734106	-1.064459	0.278572
6	-4.710127	1.309604	-1.121679
1	-5.602512	1.057758	-1.716298
1	-5.048035	1.472250	-0.093217
1	-4.346905	2.271221	-1.497766
6	-3.352648	-0.045790	-2.703459
1	-2.663078	-0.885169	-2.856726
1	-4.271520	-0.292018	-3.259009
1	-2.928689	0.835808	-3.199271
6	-0.105883	1.435455	-2.203674
1	0.671338	0.719588	-1.972469
1	-0.820366	1.010083	-2.909048
1	0.368444	2.318225	-2.647910
6	-1.742391	2.905458	-1.396418
1	-2.391080	2.479737	-2.158313
1	-2.355307	3.256610	-0.569613
1	-1.189186	3.742916	-1.833956
6	0.239149	-1.630478	-2.405950
1	1.015206	-1.171076	-3.025486
1	-0.099210	-2.561812	-2.875090
1	-0.615245	-0.969185	-2.312909
6	1.783144	-3.012037	-1.275522
1	2.100984	-3.424637	-0.322585
1	1.372437	-3.811488	-1.900073
1	2.639543	-2.586635	-1.788649
6	2.127064	1.963703	1.354924
1	2.942677	1.361063	1.726280

6	2.083936	3.276218	1.819240
1	2.823662	3.624442	2.532885
6	0.182299	3.626812	0.422213
1	-0.574317	4.306301	0.055761
6	1.097940	4.120633	1.344137
1	1.032039	5.153831	1.668286
6	-2.173120	-1.994869	1.233664
1	-2.885053	-1.336838	1.712673
6	-2.281722	-3.345777	1.546784
1	-3.024606	-3.681841	2.262988
6	-0.489432	-3.755354	0.026728
1	0.175957	-4.473263	-0.432408
6	-1.449413	-4.244327	0.903325
1	-1.520830	-5.311662	1.084473

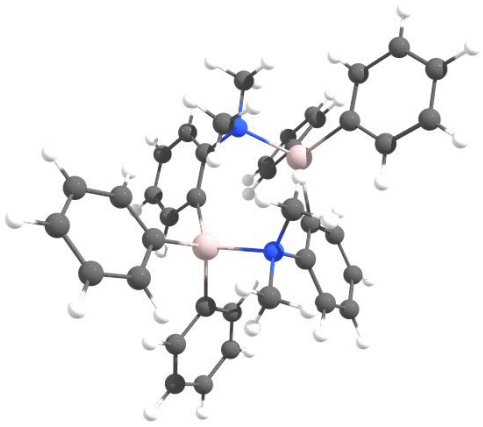

Figure S93: Computed structure of CH_3/Ph.

Data for system: **CH_3/Ph**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -2142.69122584 A.U.
Zero-point correction= 0.703307 (Hartree/Particle)
Thermal correction to Energy= 0.743120
Thermal correction to Enthalpy= 0.744065
Thermal correction to Gibbs Free Energy= 0.631215

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.993954	4.765844	1.790631
6	1.762538	5.094967	1.190571
13	-0.202473	5.026007	1.646159
7	2.995971	3.892086	2.986268
6	1.860882	5.856513	0.008224
1	0.948896	6.136940	-0.513928
6	3.070790	6.268698	-0.547343
1	3.079045	6.848061	-1.464915
6	4.215494	5.171660	1.252284
1	5.156003	4.886735	1.702822
6	4.254749	5.924133	0.082622

1	5.214078	6.219680	-0.329076
6	-1.638856	0.684100	0.009605
6	-0.354980	0.239294	-0.256962
1	-0.177503	-0.526311	-1.005308
1	-2.492520	0.282584	-0.526308
6	-1.836713	1.674327	0.966802
6	0.714752	0.792160	0.444792
1	1.711370	0.426886	0.207532
6	0.572138	1.795353	1.425065
6	-0.752039	2.217131	1.656455
1	-2.845590	2.027478	1.128620
7	-0.993006	3.329137	2.604225
13	2.392943	2.008705	2.270143
6	4.353716	3.625392	3.526174
1	4.850639	4.567811	3.778369
1	4.236030	3.031759	4.431986
1	4.950019	3.068002	2.802177
6	2.249569	4.518327	4.104392
1	1.262947	4.843321	3.789708
1	2.159319	3.793748	4.917433
1	2.797131	5.399843	4.456192
6	-2.428806	3.674614	2.763768
1	-2.838731	4.047603	1.823938
1	-2.992112	2.797971	3.099632
1	-2.496718	4.453270	3.522606
6	-0.524722	2.977349	3.966804
1	-1.157934	2.180321	4.372374
1	0.498286	2.614909	3.953444
1	-0.596045	3.862617	4.603517
6	-0.620393	6.550778	2.873855
6	-1.914220	6.989998	3.217527
6	0.437038	7.354223	3.341926
6	-2.140162	8.123128	3.996868
6	0.229880	8.490427	4.122429
6	-1.064040	8.874290	4.460621
1	-2.786829	6.450946	2.852694
1	1.461074	7.095883	3.074391
1	-3.156298	8.423410	4.235754
1	1.077611	9.079591	4.460296
1	-1.233692	9.757718	5.068544
6	-1.269930	4.988663	-0.026247
6	-1.025867	4.062160	-1.058402
6	-2.287112	5.930592	-0.259050
6	-1.763503	4.061037	-2.238973
6	-3.034612	5.940526	-1.437795
6	-2.775425	5.000696	-2.429820
1	-0.240860	3.314726	-0.937495
1	-2.498871	6.688866	0.493750
1	-1.549716	3.327140	-3.010863
1	-3.813586	6.683785	-1.582084
1	-3.353121	5.002676	-3.349452
6	3.797445	1.713830	0.899486
6	4.830396	0.781860	1.100707
6	3.793584	2.387114	-0.337422
6	5.815847	0.546575	0.140534
6	4.769702	2.161845	-1.303882
6	5.788603	1.241197	-1.064255
1	4.865573	0.211561	2.028131
1	3.009789	3.114105	-0.553368
1	6.599448	-0.181030	0.331853

1	4.736645	2.704683	-2.244285
1	6.552306	1.063093	-1.815587
6	2.498470	0.797220	3.859870
6	3.676224	0.475106	4.562849
6	1.345819	0.089429	4.251305
6	3.700583	-0.454705	5.600702
6	1.351521	-0.843477	5.287018
6	2.531738	-1.112446	5.972984
1	4.619778	0.943095	4.287524
1	0.410638	0.257930	3.718399
1	4.633306	-0.670912	6.113568
1	0.436773	-1.365170	5.553496
1	2.544275	-1.837270	6.781230

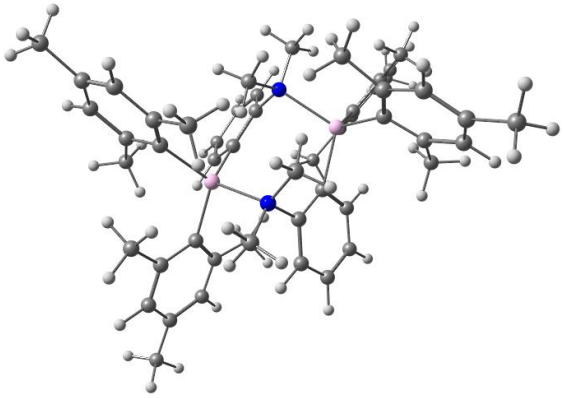

Figure S94: Computed structure of CH_3/Mes.

Data for system: **CH_3/Mes**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -2614.36239940 A.U.
Zero-point correction= 1.040653 (Hartree/Particle)
Thermal correction to Energy= 1.098880
Thermal correction to Enthalpy= 1.099824
Thermal correction to Gibbs Free Energy= 0.950513

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.926335	4.611472	1.533584
6	1.680724	5.040608	1.023228
13	-0.240421	5.203478	1.692259
7	2.988774	3.920824	2.850063
6	1.760342	5.704298	-0.216827
1	0.840711	6.055937	-0.675569
6	2.943998	5.953444	-0.905432
1	2.922743	6.481137	-1.853939
6	4.125648	4.831337	0.849590
1	5.068797	4.464367	1.227558
6	4.138009	5.508961	-0.364088
1	5.081588	5.666755	-0.876574

6	-1.419193	0.985998	-0.460264
6	-0.148251	0.459961	-0.616202
1	0.064060	-0.266614	-1.394398
1	-2.233255	0.694482	-1.116163
6	-1.652201	1.918995	0.543513
6	0.864403	0.885608	0.238568
1	1.852118	0.462066	0.080686
6	0.690848	1.812712	1.284992
6	-0.624009	2.315412	1.403795
1	-2.645054	2.338464	0.616190
7	-0.951567	3.282671	2.486004
13	2.416534	1.852013	2.373230
6	4.380344	3.852889	3.375071
1	4.808816	4.859857	3.420071
1	4.350810	3.437911	4.381149
1	4.998954	3.209386	2.753963
6	2.248195	4.772912	3.820007
1	1.179080	4.710416	3.660783
1	2.466751	4.450736	4.834671
1	2.543784	5.818488	3.691177
6	-2.421537	3.431465	2.670065
1	-2.875904	3.902751	1.801621
1	-2.873958	2.449922	2.847532
1	-2.599156	4.063437	3.538613
6	-0.456275	2.691398	3.759087
1	-0.728939	1.632817	3.803900
1	0.622274	2.758594	3.829563
1	-0.891199	3.219661	4.603368
6	-0.189493	6.813440	2.976512
6	-0.313046	6.865587	4.388272
6	0.140808	8.050656	2.359227
6	-0.042006	8.026479	5.116116
6	0.404910	9.200327	3.112466
6	0.347288	9.209456	4.498698
1	-0.156932	8.008934	6.198711
1	0.651638	10.121901	2.587408
6	-1.614208	5.335963	0.198796
6	-1.498779	4.743634	-1.084706
6	-2.806451	6.084635	0.432704
6	-2.506590	4.900175	-2.047517
6	-3.790512	6.214396	-0.546245
6	-3.657617	5.632908	-1.805678
1	-2.378919	4.420792	-3.017053
1	-4.689483	6.785586	-0.320232
6	4.077088	1.422488	1.281369
6	5.171344	0.775050	1.929440
6	4.256855	1.709473	-0.095856
6	6.340449	0.453982	1.241330
6	5.445016	1.366377	-0.757589
6	6.497799	0.735254	-0.114475
1	7.154780	-0.029555	1.778511
1	5.542164	1.613027	-1.813928
6	2.046576	0.571361	3.943600
6	1.858599	0.841621	5.322924
6	1.822850	-0.779925	3.563432
6	1.400679	-0.130068	6.215569
6	1.366288	-1.734989	4.479076
6	1.119426	-1.429455	5.809820
1	1.278026	0.133933	7.264782
1	1.213160	-2.756321	4.133703

6	0.675567	10.444304	5.296149
1	0.108511	10.475745	6.230048
1	1.739186	10.471526	5.556127
1	0.453243	11.351988	4.729571
6	-0.783511	5.690745	5.213200
1	-1.609239	5.171989	4.723636
1	0.011856	4.961601	5.405385
1	-1.147517	6.023716	6.187984
6	0.200902	8.251781	0.858785
1	1.215069	8.103748	0.475754
1	-0.467548	7.581511	0.313142
1	-0.096055	9.274491	0.610775
6	-3.086047	6.796924	1.741553
1	-4.144159	7.061544	1.811201
1	-2.833453	6.197363	2.620256
1	-2.502874	7.718949	1.829780
6	-0.320726	3.910273	-1.549500
1	0.288883	3.526580	-0.732863
1	-0.676777	3.053227	-2.126657
1	0.335882	4.491609	-2.206831
6	-4.724745	5.804687	-2.855105
1	-4.568410	5.123383	-3.694616
1	-5.719928	5.616434	-2.441980
1	-4.724617	6.826336	-3.248798
6	2.174334	2.181408	5.945193
1	2.326157	2.081179	7.022471
1	3.092049	2.600481	5.530106
1	1.370817	2.913975	5.806412
6	2.087768	-1.316018	2.171389
1	2.873724	-0.767132	1.647236
1	2.409612	-2.359287	2.232384
1	1.185437	-1.287852	1.553130
6	0.587698	-2.458482	6.772583
1	-0.506960	-2.437881	6.802828
1	0.888769	-3.467348	6.479627
1	0.947481	-2.274768	7.788251
6	5.142720	0.381293	3.393261
1	4.531731	-0.511936	3.557243
1	6.153614	0.165738	3.748369
1	4.720266	1.156099	4.038770
6	3.228064	2.387996	-0.978764
1	3.721292	3.102885	-1.642146
1	2.715019	1.657998	-1.615217
1	2.465694	2.928957	-0.420229
6	7.762287	0.359560	-0.842145
1	8.648752	0.663661	-0.278055
1	7.823932	-0.724311	-0.984100
1	7.806626	0.828515	-1.827788

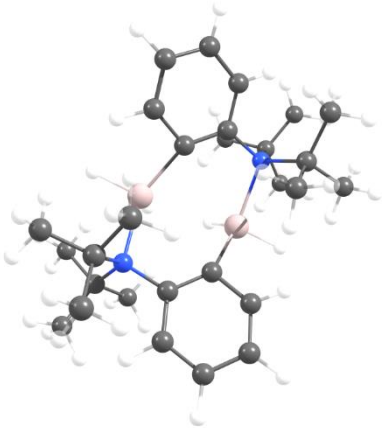

Figure S95: Computed structure of t-but/H

Data for system: **t-but/H**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1690.04246021 A.U.
Zero-point correction= 0.709692 (Hartree/Particle)
Thermal correction to Energy= 0.744507
Thermal correction to Enthalpy= 0.745451
Thermal correction to Gibbs Free Energy= 0.649737

Optimized Geometry (XYZ coordinates in Angstrom)

6	3.143690	5.057882	2.182138
6	1.735732	5.113425	2.098441
13	0.174861	4.236380	1.057917
7	3.937990	3.818730	1.881326
6	1.171495	6.345767	2.523471
1	0.093634	6.460584	2.484054
6	1.887927	7.456924	2.940884
1	1.368520	8.359930	3.245635
6	3.871044	6.202714	2.545449
1	4.944433	6.175212	2.556862
6	3.270511	7.393178	2.919410
1	3.885065	8.245235	3.191764
1	-0.854219	5.434967	1.040029
1	0.579526	3.782128	-0.389627
6	-0.617308	-0.755018	3.238778
6	0.760790	-0.813282	3.354823
1	1.255310	-1.676689	3.788471
1	-1.252047	-1.573575	3.562727
6	-1.187071	0.386330	2.699904
6	1.507830	0.247438	2.865720
1	2.585426	0.131399	2.908166
6	0.977751	1.424958	2.274042
6	-0.432457	1.486139	2.261047
1	-2.258870	0.412355	2.639257
7	-1.200207	2.682521	1.775492
13	2.607984	2.188007	1.248739
1	2.305116	2.472492	-0.265794

1	3.634103	1.001429	1.435214
6	4.867332	4.060620	0.627192
6	4.631028	3.335735	3.213744
6	-2.045801	2.301845	0.496522
6	-1.977639	3.305735	2.998314
6	5.249240	2.742981	-0.082027
1	5.791715	2.047072	0.552908
1	4.389971	2.234500	-0.514113
1	5.908397	3.013105	-0.911515
6	6.205863	4.776540	0.898137
1	6.105254	5.798798	1.256433
1	6.861505	4.218451	1.567009
1	6.719903	4.843542	-0.064558
6	4.080165	4.906481	-0.389430
1	4.626623	4.887745	-1.336445
1	3.082080	4.498775	-0.567148
1	3.983975	5.946318	-0.073392
6	3.503834	2.866713	4.144182
1	2.716851	3.620504	4.234493
1	3.057154	1.929101	3.815837
1	3.920128	2.690326	5.139780
6	5.424684	4.385149	4.027374
1	4.784293	5.138377	4.484781
1	5.905780	3.833046	4.839337
1	6.219049	4.876493	3.466246
6	5.605739	2.164446	3.004560
1	5.852385	1.777788	3.997645
1	5.170672	1.352423	2.429321
1	6.544262	2.480086	2.544837
6	-2.829257	2.350299	3.867518
1	-3.588362	1.799383	3.312824
1	-2.224787	1.652656	4.445944
1	-3.359131	2.987430	4.580863
6	-2.929725	4.445425	2.598028
1	-2.451916	5.191289	1.969502
1	-3.836162	4.080018	2.111664
1	-3.241732	4.936668	3.524248
6	-0.912323	3.875470	3.945209
1	-1.393693	4.162350	4.884132
1	-0.139524	3.136004	4.172483
1	-0.436667	4.770154	3.545600
6	-3.402551	1.616905	0.756080
1	-3.851889	1.441277	-0.225128
1	-3.330707	0.641499	1.232307
1	-4.098321	2.244619	1.313372
6	-1.197625	1.351202	-0.366937
1	-1.126703	0.352836	0.067376
1	-1.681279	1.263848	-1.343812
1	-0.188420	1.739935	-0.523021
6	-2.373763	3.532398	-0.377235
1	-2.981254	3.171426	-1.211631
1	-2.950255	4.294647	0.140896
1	-1.485590	3.990006	-0.807920

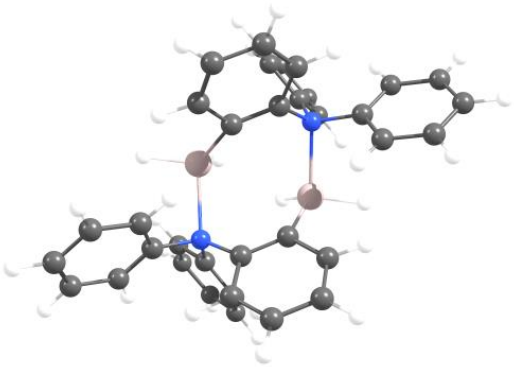

Figure S96: Computed structure of Ph/H

Data for system: **Ph/H**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=500) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -1985.37228542 A.U.
Zero-point correction= 0.574615 (Hartree/Particle)
Thermal correction to Energy= 0.608451
Thermal correction to Enthalpy= 0.609395
Thermal correction to Gibbs Free Energy= 0.509045

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.945664	4.426828	2.185560
6	1.638442	4.921001	2.065748
13	0.232930	4.573747	0.684458
7	3.423268	3.333698	1.284313
6	1.332148	6.031266	2.877722
1	0.345229	6.481227	2.787531
6	2.235987	6.604607	3.767875
1	1.944209	7.456241	4.374465
6	3.880562	5.010888	3.044368
1	4.896964	4.638801	3.088638
6	3.521698	6.088674	3.846753
1	4.258117	6.527446	4.512231
1	-0.789316	5.792078	0.657136
1	0.744260	4.065308	-0.713952
6	-1.013558	0.911334	4.610509
6	0.265975	0.379060	4.539961
1	0.615129	-0.321554	5.292023
1	-1.688059	0.635610	5.414680
6	-1.447747	1.790691	3.624397
6	1.087309	0.735278	3.473965
1	2.067545	0.267642	3.402790
6	0.704345	1.643736	2.466974
6	-0.592800	2.164241	2.584192
1	-2.460209	2.173180	3.670516
7	-1.153503	3.039960	1.509928
13	1.987989	1.666902	0.931859
1	1.358928	1.858296	-0.497530
1	3.017539	0.464734	1.089384

6	4.560059	2.622136	1.902817
6	4.325033	2.011755	3.137773
6	5.826957	2.570092	1.337197
6	5.341587	1.327834	3.783386
6	6.846044	1.874174	1.993452
6	6.611255	1.248304	3.208453
1	3.342535	2.097018	3.592137
1	6.034561	3.061782	0.395458
1	5.142472	0.855409	4.739685
1	7.831267	1.835000	1.540550
1	7.407153	0.708855	3.710513
6	3.739904	3.847717	-0.061702
6	3.812503	5.210183	-0.336192
6	3.980884	2.920552	-1.078646
6	4.095486	5.638221	-1.632992
6	4.267790	3.356940	-2.364505
6	4.319052	4.719913	-2.650084
1	3.636814	5.940575	0.443731
1	3.959841	1.856502	-0.859407
1	4.137223	6.702596	-1.838796
1	4.445504	2.625758	-3.145756
1	4.532919	5.059715	-3.657797
6	-2.240424	3.880341	2.052054
6	-3.550961	3.820148	1.597501
6	-1.907854	4.742708	3.100182
6	-4.517236	4.652423	2.169360
6	-2.872385	5.561050	3.664092
6	-4.186520	5.526058	3.194286
1	-3.833191	3.136783	0.806918
1	-0.890159	4.748451	3.478613
1	-5.537395	4.601537	1.803299
1	-2.597609	6.228584	4.474177
1	-4.941978	6.169997	3.631482
6	-1.578072	2.249189	0.339152
6	-1.912920	2.936196	-0.830425
6	-1.661377	0.860454	0.373920
6	-2.305053	2.234181	-1.961602
6	-2.050437	0.164147	-0.770170
6	-2.368574	0.842259	-1.939228
1	-1.882561	4.022230	-0.849735
1	-1.412970	0.315091	1.275873
1	-2.555688	2.780253	-2.864696
1	-2.099930	-0.919067	-0.735981
1	-2.665186	0.294276	-2.827171

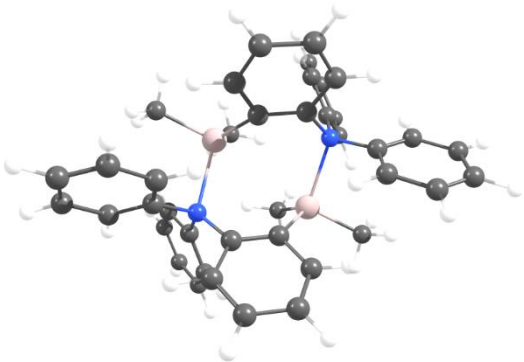

Figure S97: Computed structure of Ph/CH3

Data for system: **Ph/CH_3**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=500) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(UM062X) = -2142.65317341 A.U.
Zero-point correction= 0.693071 (Hartree/Particle)
Thermal correction to Energy= 0.733755
Thermal correction to Enthalpy= 0.734699
Thermal correction to Gibbs Free Energy= 0.623690

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.866589	4.522025	2.071967
6	1.549615	4.980746	1.939794
13	0.129707	4.659423	0.554222
7	3.388624	3.390026	1.249513
6	1.228133	6.109619	2.727826
1	0.223709	6.520475	2.658689
6	2.127099	6.742741	3.578766
1	1.816000	7.604141	4.161682
6	3.799973	5.173221	2.887953
1	4.825158	4.823238	2.927403
6	3.432871	6.274579	3.648407
1	4.169884	6.763435	4.277320
6	-0.946171	0.758037	4.551164
6	0.350552	0.270393	4.452296
1	0.734758	-0.433152	5.184421
1	-1.603978	0.440104	5.353611
6	-1.408589	1.653774	3.597296
6	1.143045	0.673799	3.383579
1	2.139511	0.245642	3.304316
6	0.722676	1.589360	2.391766
6	-0.578090	2.083194	2.554629
1	-2.428214	2.015664	3.664515
7	-1.201141	2.996651	1.550866
13	1.979261	1.559586	0.823169
6	4.425509	2.668872	2.008844
6	4.075658	2.230813	3.291038
6	5.702564	2.415173	1.523974
6	4.977408	1.508204	4.054855
6	6.604135	1.682161	2.300100
6	6.249428	1.218326	3.558066
1	3.090054	2.463285	3.680210
1	6.010913	2.776340	0.551785
1	4.683539	1.168615	5.042903
1	7.595186	1.483968	1.905096
1	6.954629	0.647320	4.152272
6	3.831645	3.859574	-0.070997
6	3.889487	5.213879	-0.395139
6	4.166628	2.910003	-1.040947
6	4.248273	5.604716	-1.684529
6	4.528359	3.308795	-2.320895
6	4.562651	4.661210	-2.653303
1	3.633710	5.968607	0.337386
1	4.149394	1.854654	-0.790553

1	4.272060	6.662496	-1.924906
1	4.775274	2.554689	-3.060860
1	4.831983	4.972491	-3.656801
6	-2.159006	3.889224	2.227139
6	-3.484079	4.038585	1.836886
6	-1.678859	4.611532	3.325440
6	-4.306239	4.944558	2.511904
6	-2.502496	5.504296	3.991278
6	-3.824272	5.685772	3.580465
1	-3.890870	3.463437	1.015661
1	-0.654069	4.464724	3.649740
1	-5.336504	5.057257	2.190462
1	-2.108342	6.062353	4.834571
1	-4.468766	6.388988	4.096758
6	-1.778357	2.235615	0.433723
6	-2.228829	2.934632	-0.690191
6	-1.853114	0.843908	0.445327
6	-2.721326	2.250664	-1.793691
6	-2.343510	0.165373	-0.669606
6	-2.773145	0.858507	-1.793222
1	-2.198835	4.018993	-0.698478
1	-1.509843	0.279489	1.302811
1	-3.056580	2.812690	-2.659084
1	-2.378897	-0.918890	-0.650585
1	-3.144720	0.323459	-2.660452
6	1.180870	1.360787	-0.971478
1	1.894562	1.535972	-1.783296
1	0.940902	0.286228	-0.994043
1	0.264808	1.895196	-1.219223
6	3.249888	0.038776	0.987310
1	3.910610	-0.027499	1.855752
1	2.616937	-0.861151	0.995746
1	3.884017	-0.064163	0.097521
6	0.724484	4.424546	-1.313341
1	0.949079	5.460687	-1.611099
1	1.613232	3.833168	-1.528334
1	-0.072290	4.076542	-1.979020
6	-1.136292	6.191391	0.495449
1	-1.866868	6.088904	-0.317079
1	-1.697378	6.469521	1.391542
1	-0.519360	7.059873	0.220331

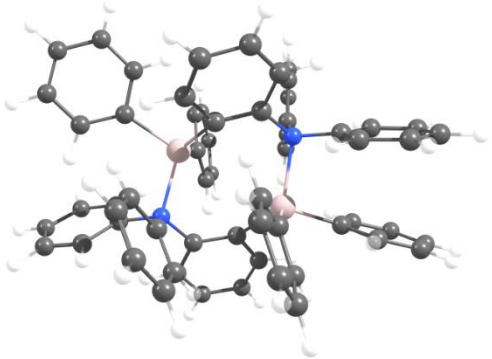

Figure S98: Computed structure of Ph/Ph

Data for system: **Ph/Ph**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -2909.58125478 A.U.
Zero-point correction= 0.913504 (Hartree/Particle)
Thermal correction to Energy= 0.966038
Thermal correction to Enthalpy= 0.966982
Thermal correction to Gibbs Free Energy= 0.830238

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.757108	5.543456	2.076905
6	1.445010	5.710691	1.597896
13	0.236007	4.691951	0.276723
7	3.389185	4.193549	2.045974
6	0.928597	7.010285	1.812879
1	-0.074813	7.238932	1.478927
6	1.636442	8.060519	2.384853
1	1.158108	9.024866	2.522397
6	3.525431	6.611510	2.554201
1	4.562712	6.458749	2.821775
6	2.968586	7.870759	2.719417
1	3.575891	8.682961	3.105502
6	-1.352737	-0.194003	1.201822
6	-0.065397	-0.532073	1.575570
1	0.256128	-1.568304	1.603266
1	-2.083942	-0.950774	0.937425
6	-1.710026	1.148913	1.171370
6	0.817182	0.478549	1.951775
1	1.790562	0.156049	2.294919
6	0.518774	1.860040	1.940065
6	-0.789268	2.150662	1.487310
1	-2.720518	1.403844	0.882825
7	-1.268421	3.561887	1.346279
13	2.025512	2.773427	3.000158
6	3.813542	3.877514	0.667483
6	4.552142	4.818392	-0.049925
6	3.593727	2.614477	0.138464
6	5.093534	4.475667	-1.282876
6	4.159651	2.266786	-1.085528
6	4.914849	3.192166	-1.794896
1	4.714188	5.807919	0.363341
1	2.962513	1.902611	0.656900
1	5.665508	5.211595	-1.838274
1	3.972472	1.280681	-1.495524
1	5.340487	2.923282	-2.756063
6	4.553021	4.054671	2.968907
6	4.454212	4.525124	4.281754
6	5.699365	3.364518	2.578852
6	5.494929	4.321218	5.178868
6	6.726066	3.145237	3.494188
6	6.635982	3.624996	4.794137
1	3.568846	5.052021	4.611045
1	5.793745	2.960103	1.579737
1	5.395300	4.699061	6.191139
1	7.597907	2.583182	3.176686
1	7.439924	3.450803	5.501389

6	-2.488350	3.633889	0.493477
6	-2.370698	3.356521	-0.869034
6	-3.743133	3.924107	1.028709
6	-3.486099	3.421449	-1.693949
6	-4.856580	3.987849	0.191293
6	-4.734678	3.748565	-1.171884
1	-1.412416	3.087865	-1.295129
1	-3.867652	4.109017	2.087682
1	-3.368173	3.221501	-2.753380
1	-5.823886	4.226072	0.621157
1	-5.602889	3.808161	-1.819465
6	-1.561179	4.172043	2.660173
6	-1.800605	5.543855	2.695371
6	-1.756178	3.399306	3.799712
6	-2.205087	6.149566	3.877502
6	-2.177898	4.011592	4.977988
6	-2.397773	5.382704	5.024114
1	-1.737329	6.120940	1.778324
1	-1.578867	2.330750	3.779612
1	-2.384088	7.219616	3.893526
1	-2.310532	3.406891	5.868181
1	-2.710446	5.852455	5.950935
6	3.422161	1.386817	3.518211
6	3.876134	1.407008	4.850589
6	4.083785	0.462214	2.683854
6	4.902775	0.585232	5.315664
6	5.112934	-0.363963	3.128510
6	5.531765	-0.305516	4.454121
1	3.433090	2.103850	5.557295
1	3.806362	0.365714	1.636224
1	5.214572	0.651743	6.354501
1	5.587195	-1.053686	2.435860
1	6.334251	-0.945590	4.808477
6	1.316152	3.643174	4.647975
6	0.963604	2.707923	5.641307
6	1.118126	4.995144	4.979209
6	0.486882	3.087166	6.895870
6	0.651312	5.388661	6.232558
6	0.340491	4.437067	7.200482
1	1.085193	1.641684	5.445047
1	1.333894	5.775316	4.252163
1	0.241740	2.329908	7.635561
1	0.521493	6.445801	6.448468
1	-0.017479	4.744586	8.178824
6	-0.672035	6.242608	-0.658043
6	0.244240	7.166274	-1.208616
6	-2.026293	6.550804	-0.874273
6	-0.146781	8.283752	-1.939972
6	-2.437545	7.675825	-1.592009
6	-1.500285	8.543457	-2.138635
1	1.312962	7.034678	-1.035163
1	-2.808094	5.913732	-0.471703
1	0.603901	8.957035	-2.343906
1	-3.498874	7.867684	-1.723037
1	-1.817539	9.415144	-2.703034
6	0.953142	3.494277	-1.176520
6	0.800644	2.106321	-1.376077
6	1.577122	4.187789	-2.231130
6	1.218921	1.466732	-2.541155
6	2.011621	3.558562	-3.398065

6	1.828933	2.190737	-3.562455
1	0.330190	1.488816	-0.616918
1	1.723573	5.262218	-2.163939
1	1.063754	0.396541	-2.649058
1	2.487313	4.144376	-4.179753
1	2.152263	1.695360	-4.473345

5. Cartesian coordinates of systems with CF_3 group

5.1 Aminoborane

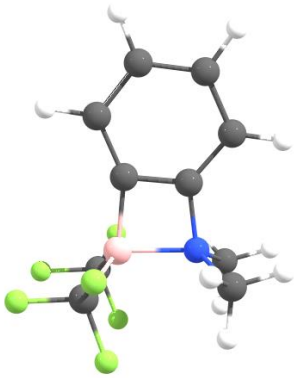

Figure S98: Computed structure of aminoalane CH_3/CF_3 (monomer).

Data for system: **CH_3/CF_3 (monomer)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1065.84180222 A.U.
Zero-point correction= 0.202039 (Hartree/Particle)
Thermal correction to Energy= 0.218225
Thermal correction to Enthalpy= 0.219169
Thermal correction to Gibbs Free Energy= 0.158143

Optimized Geometry (XYZ coordinates in Angstrom)

6	-1.325942	1.897681	0.596930
6	-0.018617	1.986282	1.036782
5	0.251052	0.470159	0.599831
7	-1.378835	0.508779	0.103576
6	0.412462	3.189262	1.584724
1	1.425816	3.324238	1.948373
6	-0.507243	4.238534	1.656787
1	-0.199569	5.189708	2.079676
6	-2.275643	2.902195	0.644071
1	-3.293426	2.785425	0.285085
6	-1.822556	4.101713	1.197661
1	-2.502188	4.944007	1.273664
6	0.484731	-0.632572	1.758729
6	1.237878	0.197221	-0.651260

6	-1.658932	0.413725	-1.351712
6	-2.345008	-0.340439	0.845635
1	-3.361388	-0.028310	0.590606
1	-2.187787	-1.380660	0.559289
1	-2.175442	-0.226776	1.913497
1	-2.697285	0.704187	-1.533184
1	-0.985619	1.075874	-1.890416
1	-1.494543	-0.615110	-1.672946
9	-0.218593	-0.387550	2.894851
9	0.119862	-1.878762	1.362331
9	1.772269	-0.709168	2.134700
9	0.947769	-0.965203	-1.289855
9	2.525322	0.119738	-0.275322
9	1.188032	1.163115	-1.605236

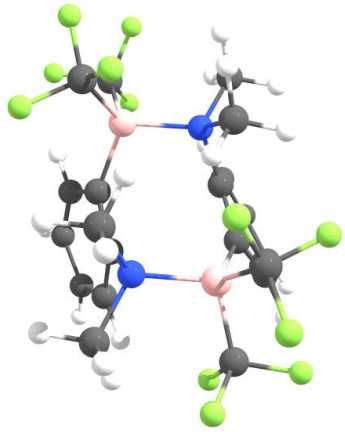

Figure S98: Computed structure of aminoalane CH_3/CF_3 (dimer).

Data for system: **CH_3/CF_3 (dimer)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -2131.63290292 A.U.
Zero-point correction= 0.412218 (Hartree/Particle)
Thermal correction to Energy= 0.443009
Thermal correction to Enthalpy= 0.443953
Thermal correction to Gibbs Free Energy= 0.354833

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.641348	4.177915	2.014514
6	1.603725	5.137176	1.838641
5	0.243327	5.159527	0.864777
7	3.093715	3.187001	0.957662
6	1.605795	6.129026	2.845508
1	0.931222	6.963562	2.764582
6	2.398882	6.117980	3.984968
1	2.315748	6.927134	4.702526
6	3.359605	4.092175	3.208368
1	4.024714	3.260773	3.380427
6	3.235432	5.041855	4.209661

1	3.809892	4.942033	5.124000
6	-0.516886	2.442773	4.540101
6	0.309309	1.336601	4.493142
1	0.421581	0.679662	5.348913
1	-1.052620	2.721739	5.440742
6	-0.682767	3.182224	3.380148
6	1.055565	1.100804	3.346401
1	1.726347	0.261071	3.400090
6	1.016675	1.880630	2.168392
6	-0.014939	2.861633	2.197117
1	-1.339598	4.036938	3.414687
7	-0.513835	3.629374	0.987112
5	2.338060	1.665612	1.164975
6	2.901769	3.806276	-0.390213
1	3.306347	4.817377	-0.364091
1	3.415333	3.201333	-1.132553
1	1.866246	3.850172	-0.657009
6	4.606636	3.105296	1.007577
1	4.970192	2.630694	1.907387
1	4.933091	2.514122	0.155253
1	4.989828	4.124034	0.939938
6	-0.372666	2.758956	-0.220962
1	0.651330	2.664427	-0.516961
1	-0.767858	1.772116	0.017776
1	-0.920419	3.207940	-1.045022
6	-2.023802	3.723711	1.081573
1	-2.387716	4.137961	0.144266
1	-2.404172	2.712401	1.229403
1	-2.353237	4.365644	1.885707
6	2.058318	0.806661	-0.254403
9	1.925058	1.494769	-1.425795
9	3.016068	-0.097458	-0.535466
9	0.916194	0.094190	-0.122721
6	3.452138	0.664171	1.904338
9	3.837333	1.051828	3.152839
9	2.959291	-0.588862	2.035977
9	4.618509	0.499853	1.237196
6	0.465046	5.725628	-0.704290
9	1.616955	6.432216	-0.764316
9	0.539190	4.821074	-1.723856
9	-0.497399	6.573878	-1.112939
6	-0.846219	6.288292	1.437870
9	-0.353493	7.541511	1.308286
9	-2.036048	6.324607	0.793394
9	-1.185458	6.149854	2.750799

5.2 Aminoalane

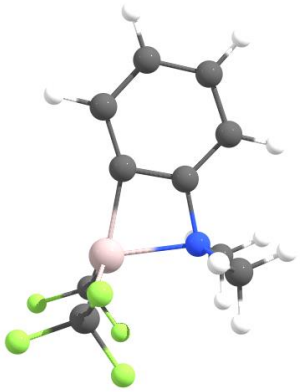

Figure S98: Computed structure of aminoalane CH_3/CF_3 (monomer).

Data for system: **CH_3/CF_3 (monomer)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -1283.41893142 A.U.
Zero-point correction= 0.194989 (Hartree/Particle)
Thermal correction to Energy= 0.213201
Thermal correction to Enthalpy= 0.214145
Thermal correction to Gibbs Free Energy= 0.147375

Optimized Geometry (XYZ coordinates in Angstrom)

6	2.906075	5.060292	2.172382
6	1.916438	6.046763	2.179936
13	1.100759	5.277597	0.578786
7	2.716993	4.130444	1.037391
6	1.975453	6.996788	3.203064
1	1.234988	7.788778	3.263205
6	2.988497	6.934439	4.156839
1	3.029663	7.674980	4.949352
6	3.931639	4.965836	3.106218
1	4.681378	4.180659	3.061903
6	3.958583	5.928575	4.110254
1	4.739284	5.898278	4.863240
6	3.841495	4.166772	0.075563
1	4.750909	3.769241	0.538379
1	3.577996	3.566667	-0.796785
1	4.008256	5.197353	-0.240572
6	2.434336	2.744742	1.474429
1	1.587489	2.752410	2.161958
1	2.175241	2.145987	0.599829
1	3.311283	2.316060	1.970885
6	1.462474	6.004160	-1.266233
6	-0.484131	4.035762	0.671956
9	-1.669907	4.543488	0.275907
9	-0.266327	2.938151	-0.108912
9	-0.691012	3.543896	1.925655

9	0.460580	6.695776	-1.848046
9	1.760645	4.984400	-2.122349
9	2.549301	6.825334	-1.300148

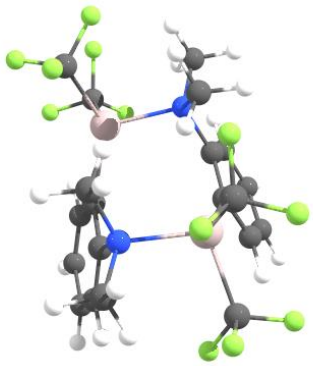

Figure S98: Computed structure of aminoalane CH_3/CF_3 (dimer).

Data for system: **CH_3/CF_3 (dimer)**

#p m062x/6-31g(d,p) scf=(maxcycles=100) int=ultrafine nosymm freq opt

--Link1--

#p m062x/def2tzvp scf=(maxcycles=100) int=ultrafine nosymm guess=read geom=check SCRF=(Solvent=benzene,SMD)

SCF Done: E(RM062X) = -2566.85978922 A.U.
Zero-point correction= 0.395571 (Hartree/Particle)
Thermal correction to Energy= 0.432060
Thermal correction to Enthalpy= 0.433004
Thermal correction to Gibbs Free Energy= 0.325661

Optimized Geometry (XYZ coordinates in Angstrom)

6	3.114562	4.247991	1.979449
6	1.951922	5.050838	2.024531
13	0.273810	5.232854	0.971000
7	3.354561	3.303436	0.854974
6	1.839575	5.883357	3.156720
1	0.984839	6.543486	3.256373
6	2.777168	5.919169	4.186112
1	2.630516	6.583393	5.030915
6	4.049359	4.257532	3.014376
1	4.915934	3.613548	2.996530
6	3.881416	5.090415	4.117053
1	4.623390	5.078823	4.908213
6	-1.112619	2.386284	4.528209
6	-0.004932	1.575055	4.690938
1	0.193358	1.086079	5.638570
1	-1.805051	2.559005	5.345104
6	-1.348364	2.990909	3.296964
6	0.868968	1.400692	3.620578
1	1.729574	0.764416	3.795192
6	0.686500	1.998671	2.356823
6	-0.477718	2.788580	2.226202
1	-2.214125	3.629702	3.206129
7	-0.786967	3.499129	0.956481
13	2.295086	1.611458	1.252422

6	2.954890	3.883991	-0.453890
1	3.469424	4.835807	-0.614526
1	3.207600	3.174156	-1.242640
1	1.890782	4.062606	-0.500177
6	4.797401	2.932105	0.702628
1	5.152343	2.360946	1.554147
1	4.886461	2.305091	-0.182661
1	5.389119	3.845103	0.588658
6	-0.431947	2.689143	-0.237658
1	0.636883	2.551769	-0.318416
1	-0.903023	1.703810	-0.179457
1	-0.762467	3.220607	-1.130862
6	-2.241613	3.822093	0.809413
1	-2.384161	4.269678	-0.172276
1	-2.821774	2.899236	0.900984
1	-2.564591	4.541980	1.554156
6	2.308299	0.648665	-0.550469
6	3.640119	0.468142	2.263906
6	0.145425	5.846078	-0.974859
6	-1.028475	6.540926	1.826431
9	4.646106	0.042249	1.455059
9	4.268655	1.099953	3.303158
9	3.113545	-0.659647	2.804500
9	2.147225	-0.676402	-0.318290
9	1.414316	0.954418	-1.529209
9	3.526208	0.770487	-1.162757
9	1.000920	5.383635	-1.925751
9	-1.096140	5.591387	-1.491797
9	0.280210	7.194048	-0.995866
9	-2.075534	6.805268	1.000401
9	-0.491999	7.751074	2.124037
9	-1.601670	6.110247	2.992512

6. References

1 Y. Zhao and D. G. Truhlar, The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-Class Functionals and 12 Other Function, *Theor. Chem. Acc.*, 2008, **120**, 215–241.

2 F. Huang, J. Jiang, M. Wen and Z.-X. Wang, Assessing the Performance of Commonly Used DFT Functionals in Studying the Chemistry of Frustrated Lewis Pairs, *J. Theor. Comput. Chem.*, 2014, **13**, 1350074.

3 G. Luchini, J. V. Alegre-Requena, I. Funes-Ardoiz and R. S. Paton, GoodVibes: Automated Thermochemistry for Heterogeneous Computational Chemistry Data, *F1000Research*, 2020, **9**, 291.

4 A. V. Marenich, C. J. Cramer and D. G. Truhlar, Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions, *J. Phys. Chem. B*, 2009, **113**, 6378–6396.

5 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G.

Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian 16, Revision C.01, Gaussian, Inc., Wallingford CT, 2016.

6 T. Lu and F. Chen, Multiwfn: A Multifunctional Wavefunction Analyzer, *J. Comput. Chem.*, 2012, **33**, 580–592.

7 D. M. Andrada and C. Foroutan-Nejad, Energy Components in Energy Decomposition Analysis (EDA) Are Path Functions; Why Does It Matter?, *Phys. Chem. Chem. Phys.*, 2020, **22**, 22459–22464.

8 M. Gimferrer, S. Danés, D. M. Andrada and P. Salvador, Merging the Energy Decomposition Analysis with the Interacting Quantum Atoms Approach, *J. Chem. Theory Comput.*, 2023, **19**, 3469–3485.

9 I. Funes-Ardoiz and R. S. Paton, GoodVibes: Version 2.0.3, *GoodVibes: version 2.0.3*, Zenodo, 2018.

10 J. Contreras-García, E. R. Johnson, S. Keinan, R. Chaudret, J.-P. Piquemal, D. N. Beratan and W. Yang, NCIPLOT: A Program for Plotting Noncovalent Interaction Regions, *J. Chem. Theory Comput.*, 2011, **7**, 625–632.