Supplementary Information

Quantum chemical analysis of 3,5-dimethyl-2,6-diphenylpyridine and its *para* amino and nitro phenyl derivatives using density functional theory

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Cartesian coordinates and thermodynamic parameters at wB97XD / Def2TZVPP level in gas phase

All coordinates are given in ångströms.
All energy is given in hartrees.
1 hartree = 627.5095 kcal/mole
The standard Gibbs energy (G°) under the conditions of 298.15 K and 1 atm in gas phase is equal to the Sum of electronic and thermal Free Energies.

Compound 1

C	-0.32980834	-1.17021522	-1.94679022
C	0.27998051	1.12390364	-0.54813187
C	-0.27998051	-1.12390364	-0.54813187
C	0.00000000	0.00000000	-2.61268359
C	0.32980834	1.17021522	-1.94679022
N	0.00000000	0.00000000	0.10466066
H	0.00000000	0.00000000	-3.69775846
C	0.73416206	2.38630892	-2.73404196
H	1.16869461	2.08952044	-3.68821994
H	1.46411044	2.98906028	-2.19662744
H	-0.12121367	3.02855968	-2.95157526
C	-0.73416206	-2.38630892	-2.73404196
H	-1.46411044	-2.98906028	-2.19662744
H	0.12121367	-3.02855968	-2.95157526
H	-1.16869461	-2.08952044	-3.68821994
C	0.56177836	2.29994766	0.31877591
C	1.08610212	4.45732095	2.01208090
C	0.00000000	3.54882469	0.07151977
C	1.37784224	2.14267632	1.43643345
C	1.64433794	3.21383451	2.27179867
C	0.25707413	4.61979944	0.91354663
H	-0.66401336	3.68297016	-0.77158765
H	1.79347217	1.16655780	1.64577051
H	2.28698977	3.07720855	3.13159634

H	-0.19681964	5.58136045	0.71293964
H	1.29101435	5.29371325	2.66717382
C	-0.56177836	-2.29994766	0.31877591
C	-1.08610212	-4.45732095	2.01208090
C	-1.37784224	-2.14267632	1.43643345
C	0.00000000	-3.54882469	0.07151977
C	-0.25707413	-4.61979944	0.91354663
C	-1.64433794	-3.21383451	2.27179867
H	-1.79347217	-1.16655780	1.64577051
H	0.66401336	-3.68297016	-0.77158765
H	0.19681964	-5.58136045	0.71293964
H	-2.28698977	-3.07720855	3.13159634
H	-1.29101435	-5.29371325	2.66717382

Zero-point correction=	0.308276 (Hartree/Particle)
Thermal correction to Energy=	0.324988
Thermal correction to Enthalpy=	0.325932
Thermal correction to Gibbs Free Energy=	0.263561
Sum of electronic and zero-point Energies=	-788.732503
Sum of electronic and thermal Energies=	-788.715791
Sum of electronic and thermal Enthalpies=	-788.714846
Sum of electronic and thermal Free Energies	-788.777218

Compound 2

C	-1.79369585	1.90183323	0.06483407
C	0.74326937	0.81823215	-0.02444099
C	-1.55655298	0.52291975	0.03013052
C	-0.67457675	2.71753976	-0.00500428
C	0.61448050	2.21368085	-0.07171193
N	-0.32419230	0.02445470	0.00724164
H	-0.81421402	3.79369882	-0.01044883
C	1.77463311	3.16011716	-0.21451378
H	1.45260513	4.07953801	-0.70287674
H	2.57900445	2.72125120	-0.80249653
H	2.19363894	3.43671462	0.75486415
C	-3.15929033	2.51952396	0.19271492
H	-3.83136011	1.89354649	0.77711359
H	-3.62521711	2.67556919	-0.78209515
H	-3.08802275	3.49264739	0.67799292
C	2.05045323	0.11477178	-0.04019199
C	4.48140034	-1.31087727	-0.06880448
C	3.13281002	0.52082086	0.73378926
C	2.20518992	-1.03200871	-0.81650746
C	3.39642074	-1.72844967	-0.84183194

C	4.32738796	-0.17650130	0.72657541
H	3.04081481	1.38274880	1.38051966
H	1.36581453	-1.38067451	-1.40269782
H	3.49222768	-2.60865392	-1.46616825
H	5.14974033	0.15915508	1.34673934
C	-2.64323736	-0.49383092	0.05023357
C	-4.62379816	-2.46266641	0.09540251
C	-2.52062254	-1.60547901	0.88051893
C	-3.76433172	-0.39199186	-0.76788043
C	-4.74649641	-1.37041482	-0.74853054
C	-3.50560583	-2.57769641	0.90902469
H	-1.63709240	-1.70025226	1.49679391
H	-3.86201650	0.44584219	-1.44477526
H	-5.60630608	-1.28071963	-1.39943516
H	-3.39897575	-3.43104035	1.56590256
H	-5.39205523	-3.22438841	0.11447561
N	5.69662695	-1.98097466	-0.12829558
H	6.29969370	-1.85652166	0.66585537
H	5.64765424	-2.93996014	-0.42472205

Zero-point correction=	0.325512 (Hartree/Particle)
Thermal correction to Energy=	0.343475
Thermal correction to Enthalpy=	0.344419
Thermal correction to Gibbs Free Energy=	0.279127
Sum of electronic and zero-point Energies=	-844.081959
Sum of electronic and thermal Energies=	-844.063996
Sum of electronic and thermal Enthalpies=	-844.063051
Sum of electronic and thermal Free Energies=	-844.128344

Compound 3

C	-0.21069532	2.40509270	-0.11430271
C	-2.16619202	0.46429993	0.02372587
C	0.07539462	1.03813232	-0.03937712
C	-1.55305141	2.75129761	-0.06325511
C	-2.56426839	1.80836577	0.02495961
N	-0.88346931	0.11837356	0.00776110
H	-1.82099834	3.80213127	-0.09213333
C	-3.99461109	2.25819617	0.13610729
H	-4.04445579	3.24592031	0.59314108
H	-4.58660307	1.57029539	0.73697492
H	-4.47108395	2.32781444	-0.84329358
C	0.82935221	3.48097103	-0.26604494
H	1.69487679	3.13279816	-0.82686280
H	1.18692422	3.83497104	0.70266793

H	0.40794909	4.33912410	-0.78829806
C	-3.12538960	-0.67169836	0.06776765
C	-4.86175653	-2.85479707	0.15443126
C	-4.23625519	-0.72715722	-0.76842130
C	-2.88721823	-1.73244275	0.93804963
C	-3.75259733	-2.81185222	0.98689738
C	-5.09717416	-1.81288148	-0.72848875
H	-4.41945952	0.07101160	-1.47493619
H	-2.01094354	-1.70354681	1.57112065
H	-3.55880031	-3.62478079	1.67410220
H	-5.95021790	-1.84623411	-1.39319360
C	1.45808410	0.48827951	-0.03641693
C	3.99094171	-0.61167645	-0.03663677
C	1.74335013	-0.63208082	-0.81509354
C	2.46620844	1.03267140	0.75506943
C	3.73685462	0.48630229	0.76289629
C	3.00948758	-1.18395952	-0.82656056
H	0.95394824	-1.07195105	-1.40753656
H	2.25509147	1.87879033	1.39296989
H	4.52255777	0.89417274	1.38013463
H	3.24334448	-2.04565841	-1.43279874
H	-5.53568648	-3.70044245	0.18924143
N	5.34243327	-1.19270527	-0.04085038
O	5.53817472	-2.15776298	-0.74772694
O	6.18157832	-0.67154587	0.66253758

Zero-point correction=	0.311692 (Hartree/Particle)
Thermal correction to Energy=	0.330673
Thermal correction to Enthalpy=	0.331618
Thermal correction to Gibbs Free Energy=	0.262549
Sum of electronic and zero-point Energies=	-993.253158
Sum of electronic and thermal Energies=	-993.234177
Sum of electronic and thermal Enthalpies=	-993.233233
Sum of electronic and thermal Free Energies=	-993.302302

Compound 4

C	0.35192106	2.58640985	-0.10255028
C	-1.80978982	0.86736909	0.01069066
C	0.48405151	1.19633224	-0.03995537
C	-0.94537471	3.07609986	-0.05083713
C	-2.0538847	2.24970252	0.02784125
N	-0.56988751	0.38669927	-0.00756234
H	-1.09659523	4.15032789	-0.06802999
C	-3.42383026	2.85665592	0.15136699

H	-3.35929575	3.84172768	0.61245789
H	-4.08322257	2.23536531	0.75493883
H	-3.89845468	2.98418135	-0.82321685
C	1.50405763	3.54357924	-0.24123347
H	2.32708523	3.10994648	-0.80660497
H	1.89760447	3.84552148	0.7312697
H	1.18007516	4.44874464	-0.75369988
C	-2.88314	-0.15620995	0.04500826
C	-4.84801527	-2.17512128	0.1091289
C	-4.03125274	-0.06866275	-0.73616078
C	-2.73107371	-1.28547905	0.847262
C	-3.69439889	-2.27233736	0.89008919
C	-4.99715409	-1.05779219	-0.71189869
H	-4.16897341	0.77224749	-1.40210458
H	-1.83316887	-1.38596809	1.44174415
H	-3.55606269	-3.13200363	1.53450601
H	-5.87607387	-0.96638546	-1.33832441
C	1.79743785	0.49653334	-0.03673868
C	4.19232415	-0.87919966	-0.03668635
C	1.96140713	-0.6401566	-0.82692633
C	2.85519987	0.91624416	0.76602672
C	4.05705509	0.23166948	0.77403756
C	3.15807567	-1.32961215	-0.83826603
H	1.13119822	-0.98227324	-1.42801238
H	2.73544536	1.7729926	1.41335727
H	4.87934573	0.54271385	1.3999518
H	3.2993857	-2.20546344	-1.45289903
N	-5.84023195	-3.14113056	0.18492662
H	-6.458422	-3.19687426	-0.60509913
H	-5.54595204	-4.04512833	0.51000106
N	5.46962796	-1.60787294	-0.04067238
O	5.56042816	-2.5814957	-0.75738874
O	6.3580502	-1.19221566	0.67260506

Zero-point correction=	0.328408 (Hartree/Particle)
Thermal correction to Energy=	0.348907
Thermal correction to Enthalpy=	0.349852
Thermal correction to Gibbs Free Energy=	0.277802
Sum of electronic and zero-point Energies=	-1048.603575
Sum of electronic and thermal Energies=	-1048.583075
Sum of electronic and thermal Enthalpies=	-1048.582131