

# Can range-separated hybrid DFT functionals predict low-lying excitations? A Tookad case study

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## Supporting Information

S1: Gas phase TDDFT calculations

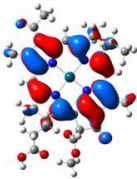

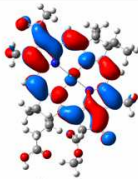

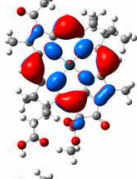


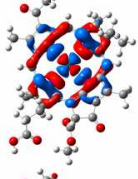
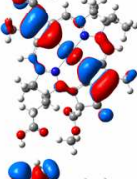



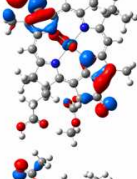
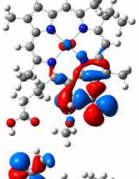
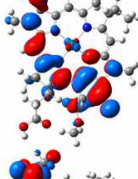
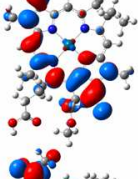
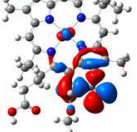

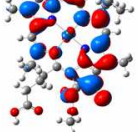

S2: Calculated molecular orbitals of Tookad with B3LYP and  $\omega$ B97XD functionals

S3: Cartesian coordinates of the optimized geometries of Tookad and Bpheid in gas phase, THF and toluene with B3LYP and M06 functionals

**Table S1:** Gas phase TDDFT calculations

Geometry Methods	TDDFT Methods	Absorptions of first two peaks (nm)			
		Tookad		Bpheid	
		Q <sub>y</sub>	Q <sub>x</sub>	Q <sub>y</sub>	Q <sub>x</sub>
B3LYP	B3LYP	659	519	649	543
B3LYP	M06HF	785	515	778	523
B3LYP	wB97XD	726	520	725	545
M06	B3LYP	654	515	647	539
M06	M06HF	777	511	767	518
M06	wB97XD	719	515	720	540

**Table S2:** Extended set of calculated molecular orbitals of Tookad with the B3LYP and  $\omega$ B97XD functionals

	B3LYP	$\omega$ B97XD		B3LYP	$\omega$ B97XD
HOMO			LUMO		
HOMO-1			LUMO+1		
HOMO-2			LUMO+2		
HOMO-3			LUMO+3		
HOMO-4			LUMO+4		

**Tables S3:** Cartesian coordinates of the optimized geometries of Tookad and Bpheid in gas phase, THF and toluene with B3LYP and M06 functionals

S3-1 Tookad-B3LYP-Gasphase  
S3-2 Tookad-B3LYP-THF  
S3-3 Tookad-B3LYP-Toluene  
S3-4 Tookad-M06-Gasphase  
S3-5 Tookad-M06-THF  
S3-6 Tookad-M06-Toluene  
S3-7 Bpheid-B3LYP-Gasphase  
S3-8 Bpheid-B3LYP-THF  
S3-9 Bpheid-B3LYP-Toluene  
S3-10 Bpheid-M06-Gasphase  
S3-11 Bpheid-M06-THF  
S3-12 Bpheid-M06-Toluene

**S3-1 Tookad-B3LYP-Gasphase**

O 1  
N 0.738364 -0.983711 -0.006571  
C 0.769324 -2.339207 -0.100167  
C 2.195832 -2.851162 -0.230555  
C 3.028455 -1.630450 0.221107  
C 2.026373 -0.497187 0.082460  
C -0.316141 -3.195245 -0.122356  
C -1.675923 -2.868437 -0.097808  
C -2.758957 -3.820402 -0.127549  
C -3.934939 -3.077426 -0.127867  
C -3.540366 -1.673958 -0.114859  
N -2.176252 -1.592203 -0.084484  
C -4.379541 -0.555795 -0.206312  
C -4.016144 0.778759 -0.197709  
C -5.030799 1.896130 -0.390424  
C -4.261041 3.122900 0.144848  
C -2.815740 2.660088 0.021114  
N -2.764018 1.285589 -0.061197  
C -1.741984 3.523307 0.006038  
C -0.385804 3.156695 -0.024826  
N 0.017786 1.833910 -0.006364  
C 1.355499 1.848299 -0.001311  
C 1.861330 3.171970 -0.018932  
C 0.764044 4.030837 -0.035399  
C 2.329074 0.846712 0.061775  
C 3.681514 1.555495 0.110047  
C 3.316581 3.109738 0.024390  
O 4.142248 4.004743 0.021322  
C 4.653050 1.174420 -0.997542  
O 5.901306 1.539618 -0.675245  
C 6.918851 1.258241 -1.653443  
C 0.746858 5.528426 -0.060354  
C -4.673005 3.460405 1.601405  
C -4.014135 4.704071 2.207030  
C -5.440435 2.033118 -1.869641  
C -5.282119 -3.687581 -0.105323  
C -6.502078 -2.901509 0.355317

C	-2.605459	-5.309434	-0.140497
C	2.510070	-3.286382	-1.675395
C	3.541998	-1.737915	1.678800
C	4.602001	-2.823224	1.902976
C	5.932683	-2.538746	1.239623
O	6.250242	-1.511375	0.676517
O	-5.429878	-4.867007	-0.425464
O	4.347067	0.631168	-2.042568
O	6.781353	-3.591253	1.356772
H	-3.347657	-5.784147	0.505959
H	-1.607137	-5.617007	0.181195
H	-2.784880	-5.711648	-1.144403
H	-7.266263	-3.619513	0.659429
H	-6.909396	-2.315042	-0.477478
H	-6.279612	-2.218446	1.179458
H	-5.439192	-0.739617	-0.313837
H	-0.076808	-4.251088	-0.184448
H	-5.929125	1.702223	0.207353
H	-5.917420	1.117829	-2.234298
H	-4.568158	2.232478	-2.501659
H	-6.149141	2.859865	-1.993507
H	-4.428447	4.909535	3.199762
H	-4.190569	5.590776	1.585506
H	-2.933374	4.579767	2.320799
H	-4.473130	2.588246	2.238003
H	-5.762629	3.599406	1.601360
H	-4.433752	4.008160	-0.479711
H	-1.966546	4.584124	0.029902
H	0.177526	5.941414	0.781464
H	0.287717	5.910056	-0.980934
H	1.765201	5.919325	-0.005439
H	4.203607	1.419432	1.064300
H	2.692164	-1.942318	2.341650
H	3.957352	-0.773713	1.987028
H	3.879158	-1.462824	-0.444487
H	1.850384	-4.098372	-1.997472
H	3.545823	-3.636087	-1.751260
H	2.386042	-2.448519	-2.369163
H	2.342768	-3.710744	0.434006
H	7.837287	1.674291	-1.240335
H	6.673177	1.732829	-2.606433
H	7.013156	0.178626	-1.792421
H	4.804758	-2.937758	2.975828
H	4.264163	-3.811003	1.568563
H	7.618490	-3.335507	0.933146
Pd	-1.057369	0.130857	-0.034994

### S3-2 Tookad-B3LYP-THF

0 1

N	0.755630	-0.991648	-0.016224
C	0.789579	-2.346075	-0.104376
C	2.216586	-2.859682	-0.216707
C	3.041379	-1.638875	0.249026
C	2.046633	-0.504117	0.070378
C	-0.297690	-3.203000	-0.140100
C	-1.655034	-2.870012	-0.129878
C	-2.740644	-3.821764	-0.187110
C	-3.913875	-3.077424	-0.188719
C	-3.519621	-1.672700	-0.146932
N	-2.154962	-1.594152	-0.105132
C	-4.360368	-0.557792	-0.224827
C	-3.998255	0.779982	-0.188538
C	-5.017759	1.896811	-0.346559
C	-4.245260	3.116979	0.200664
C	-2.800369	2.657967	0.066039

N	-2.747218	1.282125	-0.045018
C	-1.727555	3.520582	0.065571
C	-0.368426	3.157391	0.017563
N	0.036394	1.831931	-0.000045
C	1.372165	1.844561	-0.012602
C	1.879957	3.168451	-0.000652
C	0.776872	4.030240	0.019663
C	2.345035	0.838060	0.030644
C	3.697130	1.546624	0.042586
C	3.327047	3.099342	0.041216
O	4.166156	3.991027	0.081390
C	4.579101	1.249190	-1.162478
O	5.867257	1.495220	-0.888625
C	6.803699	1.330295	-1.977213
C	0.752279	5.527836	0.029304
C	-4.652981	3.438029	1.662354
C	-3.998377	4.679710	2.276546
C	-5.452178	2.058623	-1.816293
C	-5.268207	-3.668441	-0.185792
C	-6.447166	-2.923477	0.416138
C	-2.575025	-5.309329	-0.212120
C	2.547815	-3.298505	-1.656522
C	3.494498	-1.734759	1.729263
C	4.510001	-2.847419	2.016723
C	5.887331	-2.601481	1.442970
O	6.310573	-1.538718	1.027316
O	-5.449505	-4.803157	-0.638546
O	4.174970	0.874937	-2.250053
O	6.645985	-3.721594	1.463436
H	-3.422274	-5.805500	0.264606
H	-1.654288	-5.619977	0.288798
H	-2.536765	-5.680637	-1.243909
H	-7.175286	-3.660666	0.761529
H	-6.935971	-2.315838	-0.355218
H	-6.160163	-2.267217	1.240746
H	-5.419937	-0.740727	-0.337378
H	-0.059959	-4.259107	-0.201757
H	-5.905487	1.686377	0.260135
H	-5.937894	1.150399	-2.186879
H	-4.591797	2.271372	-2.460242
H	-6.162389	2.887507	-1.908855
H	-4.414810	4.875261	3.270444
H	-4.178098	5.568774	1.659872
H	-2.916865	4.560248	2.390634
H	-4.449265	2.560832	2.290896
H	-5.742499	3.573027	1.664152
H	-4.419763	4.009092	-0.412285
H	-1.953616	4.579956	0.113799
H	0.051102	5.916651	0.775958
H	0.443139	5.928477	-0.944590
H	1.744007	5.927669	0.252312
H	4.283120	1.359199	0.948302
H	2.612874	-1.906478	2.357838
H	3.922143	-0.777298	2.040617
H	3.920714	-1.487155	-0.384824
H	1.899363	-4.119477	-1.977649
H	3.586763	-3.640339	-1.717079
H	2.420316	-2.467666	-2.358608
H	2.353652	-3.718615	0.448327
H	7.777662	1.577208	-1.557662
H	6.553067	2.008644	-2.795557
H	6.788290	0.298463	-2.334134
H	4.644931	-2.950528	3.101591
H	4.164415	-3.827869	1.673266
H	7.528572	-3.495827	1.120227
Pd	-1.038681	0.127985	-0.039505

### S3-3 Tookad-B3LYP-Toluene

0 1

N	0.747497	-0.990541	-0.011265
C	0.778533	-2.345686	-0.102248
C	2.205012	-2.860245	-0.220315
C	3.033825	-1.640074	0.239754
C	2.037325	-0.505026	0.076816
C	-0.308811	-3.200691	-0.134475
C	-1.667211	-2.869164	-0.119184
C	-2.752492	-3.819428	-0.167050
C	-3.926353	-3.074199	-0.165597
C	-3.530178	-1.670745	-0.134014
N	-2.165777	-1.592448	-0.097116
C	-4.368851	-0.552925	-0.217641
C	-4.004680	0.782740	-0.193030
C	-5.020249	1.901457	-0.367505
C	-4.248057	3.123213	0.176296
C	-2.803429	2.660386	0.048604
N	-2.752466	1.285505	-0.050816
C	-1.728864	3.522020	0.043868
C	-0.371882	3.155316	0.003816
N	0.031041	1.830876	0.000832
C	1.367809	1.843037	-0.004637
C	1.876058	3.166640	-0.004353
C	0.776591	4.028019	0.001061
C	2.339682	0.837733	0.045646
C	3.693045	1.544101	0.071298
C	3.327261	3.098382	0.035825
O	4.161949	3.990113	0.055731
C	4.611763	1.213087	-1.096416
O	5.881755	1.523413	-0.803868
C	6.850793	1.321603	-1.852784
C	0.754266	5.525682	-0.001653
C	-4.659723	3.452135	1.634995
C	-4.002160	4.693549	2.246566
C	-5.441189	2.054195	-1.842086
C	-5.278359	-3.671284	-0.152830
C	-6.471941	-2.906073	0.397299
C	-2.593797	-5.307782	-0.193271
C	2.530404	-3.299217	-1.661428
C	3.510485	-1.740365	1.711470
C	4.545765	-2.840401	1.975113
C	5.901502	-2.580774	1.355996
O	6.264811	-1.544825	0.834318
O	-5.449071	-4.825268	-0.553108
O	4.249421	0.759495	-2.167294
O	6.713728	-3.660195	1.462435
H	-3.404247	-5.797433	0.350501
H	-1.638624	-5.619546	0.237384
H	-2.643066	-5.687283	-1.221258
H	-7.214960	-3.633680	0.730489
H	-6.931182	-2.307463	-0.398983
H	-6.206187	-2.238246	1.220309
H	-5.428555	-0.735003	-0.329574
H	-0.071445	-4.256883	-0.197880
H	-5.913860	1.699474	0.234020
H	-5.924401	1.144290	-2.211912
H	-4.574133	2.259383	-2.479387
H	-6.148846	2.883856	-1.949105
H	-4.419945	4.895098	3.238646
H	-4.176686	5.581627	1.626713
H	-2.921644	4.569335	2.363765
H	-4.460278	2.576905	2.267543
H	-5.749075	3.590833	1.634070
H	-4.419316	4.012648	-0.442063
H	-1.952615	4.582437	0.082213
H	0.124689	5.922475	0.803452
H	0.358013	5.918505	-0.946545

H	1.763005	5.923440	0.128234
H	4.254966	1.376169	0.996469
H	2.641186	-1.925555	2.353836
H	3.932130	-0.779570	2.021182
H	3.902791	-1.482886	-0.405573
H	1.876863	-4.116126	-1.983128
H	3.567851	-3.645322	-1.727254
H	2.405784	-2.466022	-2.360815
H	2.344661	-3.718896	0.445814
H	7.803919	1.631668	-1.426523
H	6.599710	1.933347	-2.722344
H	6.881245	0.268270	-2.139915
H	4.711735	-2.945538	3.055207
H	4.202885	-3.825583	1.639793
H	7.573992	-3.423620	1.074051
Pd	-1.046099	0.128782	-0.036566

### S3-4 Tookad-M06-Gasphase

O	1		
N	0.696970	-1.013891	-0.012926
C	0.696963	-2.364607	-0.098520
C	2.103650	-2.898852	-0.239017
C	2.951754	-1.713235	0.232358
C	1.992141	-0.564112	0.070053
C	-0.404927	-3.194046	-0.123149
C	-1.750494	-2.830804	-0.096631
C	-2.854416	-3.749474	-0.128185
C	-4.004941	-2.976808	-0.123921
C	-3.576108	-1.591762	-0.103134
N	-2.215139	-1.546824	-0.076129
C	-4.382159	-0.453038	-0.179458
C	-3.979182	0.866529	-0.169444
C	-4.952162	2.006152	-0.367681
C	-4.155679	3.194746	0.176796
C	-2.733237	2.709848	0.013370
N	-2.717740	1.337595	-0.054811
C	-1.644935	3.546642	-0.026033
C	-0.302542	3.142888	-0.062596
N	0.058400	1.815375	-0.026730
C	1.390779	1.790110	-0.027984
C	1.936425	3.091085	-0.067956
C	0.866786	3.977612	-0.091225
C	2.332652	0.765136	0.044657
C	3.692777	1.429669	0.086939
C	3.386636	2.977328	-0.037620
O	4.240136	3.837310	-0.074779
C	4.658033	0.969711	-0.980448
O	5.881618	1.429764	-0.731293
C	6.894555	1.016323	-1.644548
C	0.885423	5.464131	-0.129872
C	-4.504405	3.471126	1.647411
C	-3.767409	4.642653	2.273527
C	-5.298094	2.152023	-1.847846
C	-5.358839	-3.554701	-0.105397
C	-6.551914	-2.725487	0.304327
C	-2.741704	-5.230717	-0.146076
C	2.401260	-3.260661	-1.692722
C	3.404515	-1.833613	1.692269
C	4.523996	-2.843441	1.882318
C	5.831405	-2.404758	1.284689
O	6.047290	-1.357180	0.718701
O	-5.526630	-4.734281	-0.392531
O	4.366038	0.279928	-1.933810
O	6.784992	-3.339577	1.457987
H	-3.463748	-5.686543	0.538927
H	-1.735958	-5.568013	0.123200
H	-2.989792	-5.630099	-1.136966



H	-7.360612	-3.408573	0.575399
H	-6.897557	-2.118198	-0.542114
H	-6.331724	-2.052740	1.139785
H	-5.452587	-0.600311	-0.279768
H	-0.187232	-4.258676	-0.188511
H	-5.871240	1.837960	0.212573
H	-5.780275	1.247822	-2.236767
H	-4.388753	2.327607	-2.437748
H	-5.976328	2.999135	-2.006193
H	-4.133141	4.837950	3.287300
H	-3.912044	5.560406	1.687123
H	-2.689745	4.455960	2.343361
H	-4.319480	2.553403	2.228105
H	-5.588862	3.650765	1.696897
H	-4.327379	4.109099	-0.412587
H	-1.848075	4.616402	-0.012343
H	0.377156	5.898436	0.741370
H	0.380583	5.851534	-1.024372
H	1.915296	5.831864	-0.137691
H	4.204567	1.304758	1.053827
H	2.542098	-2.120325	2.312321
H	3.738213	-0.852464	2.056036
H	3.832917	-1.573218	-0.407581
H	1.706973	-4.018342	-2.073949
H	3.424205	-3.645719	-1.789683
H	2.322160	-2.367477	-2.326854
H	2.237703	-3.785522	0.399129
H	7.802953	1.534745	-1.335819
H	6.626678	1.288906	-2.669650
H	7.029351	-0.068318	-1.578467
H	4.708497	-3.046637	2.945685
H	4.277168	-3.822941	1.446257
H	7.601026	-2.993664	1.063447
Pd	-1.054296	0.141216	-0.037592

### S3-5 Tookad-M06-THF

O 1			
N	0.699534	-1.019647	-0.009590
C	0.703176	-2.370118	-0.078167
C	2.109577	-2.909772	-0.192157
C	2.957601	-1.711162	0.247769
C	1.996780	-0.566242	0.070852
C	-0.400004	-3.201544	-0.108873
C	-1.743552	-2.834882	-0.098186
C	-2.849115	-3.754964	-0.145350
C	-3.997757	-2.982303	-0.142605
C	-3.571265	-1.595541	-0.109492
N	-2.209485	-1.551527	-0.076624
C	-4.380824	-0.462467	-0.186451
C	-3.979797	0.860980	-0.172047
C	-4.957454	1.996539	-0.360727
C	-4.161404	3.188132	0.178406
C	-2.738640	2.706750	0.013918
N	-2.720004	1.331117	-0.057328
C	-1.652047	3.543758	-0.024121
C	-0.306256	3.143700	-0.063582
N	0.058151	1.813923	-0.036120
C	1.389058	1.789261	-0.040175
C	1.933320	3.091348	-0.071201
C	0.857240	3.979358	-0.086402
C	2.331831	0.762186	0.033014
C	3.689634	1.431388	0.075894
C	3.375676	2.977013	-0.028685
O	4.235717	3.840699	-0.042855
C	4.644179	0.997382	-1.011883
O	5.879714	1.417482	-0.756617
C	6.878159	1.037955	-1.707738

C	0.866743	5.466279	-0.109695
C	-4.508028	3.468373	1.649069
C	-3.778372	4.648359	2.267764
C	-5.317469	2.141156	-1.837894
C	-5.355816	-3.545971	-0.126825
C	-6.511373	-2.754770	0.426549
C	-2.728201	-5.235304	-0.168789
C	2.412814	-3.328331	-1.628914
C	3.424034	-1.804153	1.705836
C	4.536758	-2.818470	1.907846
C	5.845059	-2.400276	1.300891
O	6.067165	-1.352683	0.730956
O	-5.551362	-4.690808	-0.530467
O	4.332167	0.361818	-1.998729
O	6.786830	-3.342856	1.468040
H	-3.520619	-5.704360	0.421987
H	-1.759231	-5.571876	0.212216
H	-2.844283	-5.621068	-1.189403
H	-7.273299	-3.457593	0.773490
H	-6.964178	-2.150058	-0.369641
H	-6.220477	-2.086671	1.242506
H	-5.451315	-0.611446	-0.288424
H	-0.182380	-4.266618	-0.163050
H	-5.870285	1.822237	0.226162
H	-5.800633	1.235605	-2.222123
H	-4.415564	2.324601	-2.436919
H	-6.001413	2.985084	-1.984686
H	-4.145396	4.844919	3.280835
H	-3.930676	5.560807	1.675644
H	-2.698837	4.471423	2.338021
H	-4.317659	2.554578	2.234373
H	-5.592963	3.641542	1.697567
H	-4.335570	4.099829	-0.412995
H	-1.857210	4.612844	-0.006574
H	0.350025	5.886669	0.762892
H	0.361818	5.859409	-1.001251
H	1.892465	5.844976	-0.108918
H	4.205725	1.294296	1.038415
H	2.565957	-2.073979	2.338402
H	3.767166	-0.818953	2.048605
H	3.834087	-1.582726	-0.401548
H	1.739017	-4.121452	-1.972032
H	3.444465	-3.692643	-1.707891
H	2.305191	-2.469412	-2.305176
H	2.237047	-3.773301	0.476569
H	7.817066	1.443999	-1.331555
H	6.649121	1.456646	-2.691694
H	6.933641	-0.052487	-1.776714
H	4.720680	-2.999248	2.975014
H	4.280526	-3.804310	1.493265
H	7.611540	-3.018569	1.070030
Pd	-1.052573	0.137590	-0.041467

### S3-6 Tookad-M06-Toluene

O 1			
N	0.698925	-1.015876	-0.004660
C	0.702146	-2.366883	-0.076524
C	2.109112	-2.903978	-0.199050
C	2.957552	-1.707029	0.243856
C	1.994349	-0.562302	0.074635
C	-0.399722	-3.198184	-0.103092
C	-1.744786	-2.834405	-0.089639
C	-2.848176	-3.754960	-0.132037
C	-3.998585	-2.983398	-0.134026
C	-3.572640	-1.597170	-0.107472
N	-2.211543	-1.551191	-0.072814

C	-4.381848	-0.462484	-0.190258
C	-3.981509	0.859396	-0.178088
C	-4.956824	1.996002	-0.377131
C	-4.164693	3.186584	0.169705
C	-2.740866	2.705159	0.011605
N	-2.721728	1.331425	-0.057969
C	-1.654331	3.543572	-0.024006
C	-0.309868	3.143353	-0.060186
N	0.054618	1.815287	-0.028589
C	1.386235	1.792057	-0.031493
C	1.929547	3.094521	-0.066728
C	0.855529	3.980297	-0.085724
C	2.329730	0.767321	0.041010
C	3.687662	1.436149	0.082711
C	3.375965	2.981912	-0.030865
O	4.232177	3.844679	-0.056359
C	4.648956	0.989577	-0.994085
O	5.876295	1.435643	-0.741787
C	6.889101	1.027933	-1.662162
C	0.866332	5.467008	-0.117090
C	-4.519363	3.463176	1.638974
C	-3.789407	4.638702	2.265746
C	-5.300824	2.141636	-1.857910
C	-5.354716	-3.553093	-0.119815
C	-6.525222	-2.747658	0.384788
C	-2.728140	-5.235600	-0.149697
C	2.410036	-3.309351	-1.640148
C	3.430567	-1.805078	1.699061
C	4.547325	-2.817365	1.890497
C	5.849225	-2.396608	1.269870
O	6.064611	-1.352145	0.694513
O	-5.539884	-4.710794	-0.484340
O	4.349584	0.320868	-1.961507
O	6.795271	-3.337930	1.432674
H	-3.507880	-5.701007	0.460721
H	-1.750565	-5.569998	0.211381
H	-2.871152	-5.628089	-1.164218
H	-7.302041	-3.443926	0.710903
H	-6.945714	-2.147003	-0.431940
H	-6.257427	-2.073715	1.204358
H	-5.451642	-0.612411	-0.297316
H	-0.181374	-4.263193	-0.159159
H	-5.876076	1.823793	0.200983
H	-5.780139	1.236557	-2.248147
H	-4.391761	2.322217	-2.446762
H	-5.981753	2.986629	-2.014179
H	-4.160130	4.833268	3.277828
H	-3.935961	5.554386	1.676871
H	-2.711034	4.457220	2.340191
H	-4.333802	2.547072	2.222063
H	-5.604367	3.638945	1.683065
H	-4.335864	4.099847	-0.420799
H	-1.859911	4.612726	-0.008623
H	0.350562	5.893231	0.753440
H	0.362810	5.855431	-1.011687
H	1.893037	5.843049	-0.118342
H	4.202215	1.304293	1.047092
H	2.576106	-2.078601	2.335346
H	3.773550	-0.820238	2.043242
H	3.830880	-1.574955	-0.408768
H	1.726317	-4.088611	-1.995638
H	3.437585	-3.684851	-1.723387
H	2.317311	-2.439294	-2.303881
H	2.240516	-3.771970	0.464059
H	7.801220	1.533173	-1.343954
H	6.625130	1.320639	-2.682275
H	7.014969	-0.058226	-1.611194
H	4.743106	-3.000784	2.955261
H	4.289099	-3.803203	1.476433
H	7.612955	-3.008745	1.025520

Pd -1.054613 0.138552 -0.036678

### S3-7 Bpheid-B3LYP-Gasphase

0 1

C	3.016273	3.209547	0.059490
C	1.558743	3.207988	0.018538
C	1.108088	1.867307	0.045118
C	2.128933	0.904844	0.108819
C	3.445372	1.682601	0.140298
N	-0.242065	1.880822	0.026766
C	-0.692790	3.194722	-0.006933
C	0.450053	4.059014	-0.015665
C	-2.061448	3.523272	-0.006711
C	-3.124597	2.628517	0.001377
C	-4.592177	3.049404	0.060380
C	-5.298357	1.749840	-0.396287
C	-4.200029	0.707012	-0.184342
N	-2.987663	1.270641	-0.037480
C	-4.488009	-0.661390	-0.195977
C	-3.629106	-1.764398	-0.100407
C	-3.954637	-3.177012	-0.119823
C	-2.753564	-3.895266	-0.101648
C	-1.682848	-2.942806	-0.053353
N	-2.259173	-1.690197	-0.044248
C	-0.311248	-3.220818	-0.047279
C	0.772986	-2.340274	-0.010336
C	2.218051	-2.828899	-0.097702
C	3.016312	-1.543315	0.245504
C	1.934277	-0.471487	0.134742
N	0.684603	-1.001296	0.063283
C	2.553251	-3.393908	-1.490853
C	3.650420	-1.569467	1.657644
C	4.747989	-2.623225	1.850102
C	-2.575869	-5.381934	-0.112259
C	-5.284669	-3.830291	-0.123276
O	-5.390832	-5.003571	-0.475381
C	-5.763510	1.792176	-1.864104
C	-5.056039	3.479850	1.475650
C	-4.474681	4.798169	1.996886
C	0.434264	5.556297	-0.056422
C	4.417436	1.353338	-0.984988
O	4.111301	0.848988	-2.048159
O	3.794846	4.145477	0.053951
C	-6.528539	-3.094030	0.350807
O	5.662148	1.723105	-0.653504
C	6.680664	1.488829	-1.644709
H	-3.312025	-5.869453	0.531089
H	-1.574359	-5.669384	0.216641
H	-2.741553	-5.787291	-1.116550
H	-7.266536	-3.842289	0.646155
H	-6.957686	-2.511360	-0.473375
H	-6.327333	-2.414176	1.182645
H	-5.536453	-0.897934	-0.313003
H	-1.729774	-0.829306	-0.055095
H	-0.058348	-4.274636	-0.092968
H	-6.165404	1.529870	0.238753
H	-6.189719	0.832366	-2.173834
H	-4.925936	2.018009	-2.533166
H	-6.529460	2.563472	-2.002771
H	-4.927816	5.060713	2.958718
H	-4.673905	5.623306	1.301952
H	-3.393340	4.737164	2.149222
H	-4.828838	2.670684	2.182412
H	-6.150616	3.564256	1.444386
H	-4.787979	3.876446	-0.634367

H	-2.299397	4.581271	-0.017831
H	-0.123452	5.976956	0.788915
H	-0.037899	5.926881	-0.974415
H	1.453437	5.946011	-0.019331
H	3.985784	1.567237	1.086674
H	-0.877045	1.093317	0.036353
H	2.862352	-1.757932	2.397229
H	4.068690	-0.585138	1.888113
H	3.805174	-1.362153	-0.490511
H	1.921542	-4.254355	-1.734771
H	3.598942	-3.718233	-1.534913
H	2.403861	-2.632682	-2.263631
H	2.388411	-3.616523	0.647221
H	7.590362	1.919965	-1.228230
H	6.415722	1.976761	-2.585338
H	6.801646	0.415153	-1.803710
H	5.045909	-2.668708	2.905925
H	4.400359	-3.633602	1.606759
C	6.011574	-2.365729	1.058736
O	6.874473	-3.410238	1.148812
O	6.272848	-1.365417	0.423427
H	7.669086	-3.172107	0.641151

### S3-8 Bpheid-B3LYP-THF

0 1

C	3.045793	3.166947	0.061868
C	1.595284	3.183056	0.020257
C	1.132870	1.845167	0.013127
C	2.146209	0.870593	0.057750
C	3.467663	1.638015	0.056467
N	-0.215524	1.870890	0.012776
C	-0.657208	3.190992	0.022410
C	0.487947	4.045634	0.027272
C	-2.026288	3.527441	0.046650
C	-3.093398	2.639876	0.046137
C	-4.558308	3.063291	0.122054
C	-5.273595	1.772129	-0.345609
C	-4.175221	0.725033	-0.170438
N	-2.960567	1.278620	-0.021143
C	-4.465930	-0.645891	-0.208418
C	-3.610381	-1.748975	-0.130698
C	-3.947825	-3.160015	-0.176484
C	-2.757368	-3.890306	-0.162699
C	-1.675234	-2.947399	-0.092988
N	-2.239065	-1.689348	-0.069889
C	-0.309698	-3.243993	-0.077625
C	0.781257	-2.367871	-0.030286
C	2.224910	-2.861298	-0.092099
C	3.017072	-1.577511	0.271760
C	1.946976	-0.501705	0.105539
N	0.693114	-1.029185	0.029210
C	2.584792	-3.425963	-1.479226
C	3.571123	-1.590835	1.718991
C	4.653706	-2.644146	1.982121
C	-2.582133	-5.377051	-0.186515
C	-5.291276	-3.783384	-0.193996
O	-5.442000	-4.905151	-0.683326
C	-5.766449	1.839740	-1.803634
C	-5.011598	3.479276	1.545327
C	-4.423999	4.790958	2.076134
C	0.475300	5.543443	0.034215
C	4.351856	1.375712	-1.156441
O	3.955275	0.981057	-2.238965
O	3.843431	4.094311	0.104902
C	-6.484458	-3.085501	0.432695

O	5.629275	1.679830	-0.893197
C	6.564984	1.546719	-1.986939
H	-3.422306	-5.879406	0.295607
H	-1.657425	-5.678078	0.312063
H	-2.545115	-5.748816	-1.217514
H	-7.184993	-3.850646	0.774124
H	-7.000771	-2.482596	-0.324075
H	-6.208213	-2.432846	1.263445
H	-5.515544	-0.878922	-0.326230
H	-1.699267	-0.834914	-0.072999
H	-0.066358	-4.300009	-0.121875
H	-6.128791	1.540123	0.300166
H	-6.203168	0.886732	-2.119391
H	-4.942234	2.076856	-2.485396
H	-6.532231	2.615632	-1.910448
H	-4.874015	5.044687	3.041834
H	-4.622793	5.621840	1.388413
H	-3.342122	4.726715	2.224792
H	-4.784251	2.662085	2.242870
H	-6.105506	3.567278	1.518955
H	-4.755662	3.898819	-0.560959
H	-2.257383	4.586731	0.062870
H	-0.129221	5.936641	0.859349
H	0.053516	5.943287	-0.895873
H	1.489241	5.934109	0.138568
H	4.069296	1.469684	0.955332
H	-0.859618	1.090107	0.011370
H	2.741711	-1.774919	2.411883
H	3.974403	-0.604813	1.967150
H	3.847007	-1.415027	-0.423785
H	1.961938	-4.290700	-1.729323
H	3.632358	-3.745257	-1.500805
H	2.443702	-2.668586	-2.257790
H	2.379008	-3.650720	0.652565
H	7.530501	1.834811	-1.574699
H	6.282241	2.209935	-2.806977
H	6.588759	0.513173	-2.337538
H	4.876203	-2.684361	3.056634
H	4.325509	-3.653986	1.715677
C	5.970383	-2.376106	1.289447
O	6.782769	-3.458420	1.322878
O	6.309282	-1.326674	0.775246
H	7.625096	-3.217547	0.898263

### S3-9 Bpheid-B3LYP-Toluene

O 1			
C	3.026352	3.190595	0.046977
C	1.572438	3.196436	0.011307
C	1.117174	1.856659	0.029933
C	2.135155	0.889171	0.086957
C	3.453462	1.663353	0.103921
N	-0.232199	1.875290	0.021616
C	-0.679491	3.191991	0.001603
C	0.463836	4.052453	-0.007347
C	-2.048272	3.524494	0.013448
C	-3.113514	2.633382	0.021910
C	-4.579578	3.055872	0.089642
C	-5.290850	1.759411	-0.368788
C	-4.192092	0.714813	-0.174125
N	-2.978532	1.273767	-0.027224
C	-4.480675	-0.654993	-0.198017
C	-3.622700	-1.757632	-0.111651
C	-3.953270	-3.169630	-0.146623
C	-2.756833	-3.893198	-0.131425
C	-1.681163	-2.944949	-0.069962
N	-2.252179	-1.689960	-0.052317

C	-0.312205	-3.231443	-0.058229
C	0.775276	-2.353028	-0.015152
C	2.219626	-2.844389	-0.088851
C	3.015459	-1.558954	0.260834
C	1.938677	-0.485410	0.125071
N	0.686940	-1.014139	0.051788
C	2.566973	-3.414462	-1.476953
C	3.616974	-1.578753	1.687891
C	4.712683	-2.628601	1.907630
C	-2.579362	-5.379726	-0.152872
C	-5.289690	-3.808053	-0.159373
O	-5.418608	-4.955347	-0.588301
C	-5.771870	1.811044	-1.831272
C	-5.036625	3.482280	1.508530
C	-4.450638	4.797740	2.031761
C	0.447392	5.549979	-0.033229
C	4.397070	1.357441	-1.051714
O	4.061173	0.894425	-2.126443
O	3.813736	4.123673	0.048334
C	-6.507639	-3.091607	0.399233
O	5.653109	1.703209	-0.740711
C	6.645862	1.509050	-1.769362
H	-3.374445	-5.878354	0.404918
H	-1.614917	-5.674202	0.267882
H	-2.636950	-5.764286	-1.177734
H	-7.225595	-3.848344	0.721962
H	-6.986129	-2.499296	-0.390136
H	-6.264704	-2.425224	1.230067
H	-5.529472	-0.890520	-0.315980
H	-1.718254	-0.831840	-0.059891
H	-0.063455	-4.286221	-0.104045
H	-6.151023	1.535115	0.273609
H	-6.204100	0.854066	-2.141304
H	-4.941837	2.040465	-2.508464
H	-6.537699	2.584702	-1.954829
H	-4.901243	5.057855	2.995444
H	-4.649477	5.624764	1.339196
H	-3.368991	4.734327	2.181694
H	-4.809378	2.670297	2.212089
H	-6.130828	3.569340	1.480404
H	-4.776789	3.885507	-0.601048
H	-2.282844	4.583246	0.011366
H	-0.107295	5.960961	0.818510
H	-0.029835	5.928594	-0.945077
H	1.465386	5.942309	0.002950
H	4.015270	1.531818	1.035063
H	-0.870810	1.090444	0.028531
H	2.812468	-1.769194	2.408418
H	4.025605	-0.592665	1.927067
H	3.821900	-1.387100	-0.458621
H	1.941290	-4.279456	-1.719771
H	3.614346	-3.734233	-1.509552
H	2.419425	-2.658946	-2.255783
H	2.381766	-3.630151	0.658999
H	7.579076	1.868762	-1.338524
H	6.384913	2.083627	-2.660717
H	6.721336	0.448994	-2.019774
H	4.981973	-2.670372	2.971174
H	4.375514	-3.640048	1.655969
C	5.996051	-2.362473	1.152901
O	6.845075	-3.416900	1.227325
O	6.281132	-1.342319	0.557377
H	7.658696	-3.176569	0.750618

### S3-10 Bpheid-M06-Gasphase

C	3.124165	3.041382	0.014125
C	1.669620	3.106599	-0.018918
C	1.164947	1.792898	0.023497
C	2.142137	0.796399	0.097007
C	3.478979	1.510863	0.112151
N	-0.178445	1.854807	0.010067
C	-0.572288	3.180718	-0.033228
C	0.596881	3.995644	-0.055391
C	-1.923429	3.558038	-0.024662
C	-3.005514	2.695778	0.000588
C	-4.446466	3.155362	0.095478
C	-5.185942	1.909023	-0.403684
C	-4.144370	0.829166	-0.176430
N	-2.912702	1.336572	-0.034048
C	-4.495190	-0.519727	-0.195015
C	-3.682525	-1.649793	-0.101455
C	-4.056285	-3.041624	-0.126932
C	-2.888316	-3.800868	-0.097601
C	-1.788554	-2.891916	-0.041015
N	-2.315369	-1.621651	-0.034150
C	-0.435754	-3.221956	-0.027711
C	0.669916	-2.375391	0.010735
C	2.088984	-2.903876	-0.080544
C	2.915206	-1.657609	0.274565
C	1.884828	-0.561868	0.135228
N	0.618032	-1.038525	0.069862
C	2.400815	-3.418185	-1.483194
C	3.491090	-1.703831	1.693574
C	4.642892	-2.685144	1.831189
C	-2.765296	-5.281754	-0.103112
C	-5.400547	-3.647862	-0.144580
O	-5.537411	-4.822820	-0.459803
C	-5.551567	1.989845	-1.883974
C	-4.850031	3.505346	1.535670
C	-4.176507	4.739421	2.111120
C	0.626612	5.481970	-0.103603
C	4.427746	1.100411	-0.992099
O	4.137796	0.398450	-1.935828
O	3.939577	3.937178	-0.009271
C	-6.614610	-2.851777	0.264505
O	5.632675	1.626318	-0.785394
C	6.632497	1.272313	-1.738318
H	-3.500282	-5.739192	0.566280
H	-1.764455	-5.607055	0.196020
H	-2.982757	-5.689031	-1.097381
H	-7.406710	-3.557159	0.526627
H	-6.971518	-2.249522	-0.580626
H	-6.415800	-2.177427	1.103609
H	-5.557039	-0.706674	-0.319374
H	-1.754544	-0.778637	-0.042466
H	-0.214974	-4.287378	-0.069760
H	-6.092738	1.713028	0.188196
H	-5.986482	1.049982	-2.243549
H	-4.656964	2.195829	-2.486536
H	-6.276226	2.792795	-2.064339
H	-4.583703	4.983624	3.098085
H	-4.332585	5.612760	1.463255
H	-3.096047	4.597836	2.227645
H	-4.647713	2.631366	2.174907
H	-5.941059	3.646095	1.546229
H	-4.630407	4.028748	-0.550448
H	-2.133427	4.626277	-0.040871
H	0.119168	5.923700	0.763832
H	0.124403	5.864752	-1.001161
H	1.657627	5.845242	-0.112570
H	4.028508	1.383912	1.057826
H	-0.842703	1.089825	0.032810
H	2.689404	-1.979832	2.394444
H	3.835926	-0.704636	1.991254
H	3.734412	-1.504247	-0.441626



H	1.744997	-4.248104	-1.771158
H	3.440590	-3.764607	-1.544176
H	2.275003	-2.610890	-2.216801
H	2.239549	-3.715397	0.649192
H	7.526276	1.826046	-1.449658
H	6.319327	1.550548	-2.748705
H	6.817064	0.194308	-1.696105
H	4.915795	-2.843091	2.883354
H	4.382304	-3.684617	1.452560
C	5.888860	-2.243206	1.118392
O	6.856911	-3.176344	1.200375
O	6.051145	-1.191825	0.542805
H	7.633729	-2.823992	0.737846

### S3-11 Bpheid-M06-THF

O 1			
C	3.096587	3.057038	0.042278
C	1.649544	3.115429	-0.012453
C	1.152707	1.798568	0.023230
C	2.136310	0.804431	0.104990
C	3.465935	1.531595	0.134127
N	-0.189707	1.853012	-0.001156
C	-0.592512	3.179277	-0.045932
C	0.566336	4.000681	-0.057366
C	-1.948917	3.549015	-0.044829
C	-3.026072	2.684814	-0.017073
C	-4.469197	3.135154	0.071249
C	-5.202517	1.877299	-0.409027
C	-4.151391	0.809158	-0.182624
N	-2.924147	1.321111	-0.042330
C	-4.491917	-0.546764	-0.197230
C	-3.668572	-1.663971	-0.101566
C	-4.034205	-3.059699	-0.133068
C	-2.866791	-3.813648	-0.107987
C	-1.767680	-2.898055	-0.044339
N	-2.300177	-1.630174	-0.034083
C	-0.417945	-3.227979	-0.023561
C	0.686577	-2.374018	0.022360
C	2.106482	-2.899253	-0.042903
C	2.927475	-1.642306	0.289416
C	1.891667	-0.552954	0.147845
N	0.623952	-1.039537	0.075404
C	2.435588	-3.458886	-1.423946
C	3.528538	-1.675585	1.698836
C	4.673463	-2.665985	1.826714
C	-2.731079	-5.293088	-0.116887
C	-5.380807	-3.658401	-0.142814
O	-5.540125	-4.797999	-0.570565
C	-5.586140	1.939251	-1.885956
C	-4.875910	3.505468	1.505743
C	-4.215517	4.756447	2.059607
C	0.576800	5.487520	-0.100989
C	4.426573	1.148101	-0.969128
O	4.142679	0.477640	-1.940036
O	3.914273	3.959309	0.038708
C	-6.558297	-2.906574	0.415930
O	5.631456	1.663755	-0.741439
C	6.644127	1.342979	-1.700041
H	-3.520724	-5.765220	0.474623
H	-1.761396	-5.613745	0.274566
H	-2.836351	-5.689049	-1.134074
H	-7.298255	-3.634485	0.758128
H	-7.029468	-2.311826	-0.376855
H	-6.286985	-2.234425	1.234901
H	-5.552760	-0.743302	-0.320208
H	-1.743242	-0.784771	-0.047233

H	-0.194370	-4.292750	-0.059806
H	-6.100630	1.677263	0.193519
H	-6.022080	0.993784	-2.229078
H	-4.701212	2.146392	-2.502463
H	-6.317531	2.736398	-2.062118
H	-4.630165	5.014841	3.039837
H	-4.376866	5.614430	1.393204
H	-3.133981	4.628911	2.184091
H	-4.667650	2.644468	2.160685
H	-5.967667	3.636475	1.511198
H	-4.658100	3.997066	-0.587439
H	-2.163095	4.616157	-0.065913
H	0.068733	5.918352	0.771158
H	0.061324	5.866006	-0.992363
H	1.600436	5.869776	-0.116587
H	4.006607	1.402025	1.084317
H	-0.851102	1.085137	0.018883
H	2.738870	-1.939273	2.416992
H	3.886696	-0.677245	1.981837
H	3.735404	-1.491343	-0.440986
H	1.794830	-4.308433	-1.686376
H	3.480035	-3.793737	-1.459395
H	2.304587	-2.681876	-2.189240
H	2.248685	-3.688800	0.710798
H	7.531808	1.893847	-1.390052
H	6.336224	1.650479	-2.702829
H	6.838052	0.266571	-1.684195
H	4.976076	-2.788704	2.875301
H	4.390939	-3.673947	1.491320
C	5.901267	-2.257897	1.066511
O	6.832359	-3.225955	1.076859
O	6.075916	-1.193992	0.511505
H	7.609360	-2.901393	0.592062

### S3-12 Bpheid-M06-Toluene

0 1

C	3.106574	3.051986	0.035003
C	1.655816	3.112551	-0.010690
C	1.156578	1.796378	0.026745
C	2.138066	0.802177	0.104441
C	3.470432	1.524607	0.127595
N	-0.186367	1.852906	0.006351
C	-0.586268	3.178445	-0.037882
C	0.576705	3.998308	-0.052560
C	-1.940154	3.551084	-0.035550
C	-3.019486	2.687283	-0.011125
C	-4.462055	3.141442	0.076319
C	-5.196452	1.888164	-0.413778
C	-4.149722	0.815301	-0.183630
N	-2.920928	1.326091	-0.039900
C	-4.493497	-0.537495	-0.199421
C	-3.673523	-1.659577	-0.101907
C	-4.041850	-3.053434	-0.130975
C	-2.873736	-3.809202	-0.104273
C	-1.775229	-2.896051	-0.042469
N	-2.305875	-1.627376	-0.033825
C	-0.423787	-3.225561	-0.023541
C	0.680898	-2.374834	0.019747
C	2.100761	-2.901272	-0.054287
C	2.923762	-1.647362	0.283555
C	1.889045	-0.556157	0.144286
N	0.622433	-1.039156	0.075060
C	2.424026	-3.448640	-1.441569
C	3.518691	-1.684330	1.695270
C	4.665981	-2.671888	1.825018
C	-2.741931	-5.289205	-0.112638

C	-5.387654	-3.654390	-0.142291
O	-5.541650	-4.804575	-0.538024
C	-5.568133	1.957873	-1.893277
C	-4.871082	3.503531	1.512107
C	-4.206737	4.747735	2.076368
C	0.592451	5.484949	-0.098318
C	4.425285	1.131966	-0.977825
O	4.137842	0.449816	-1.938183
O	3.922791	3.951685	0.024136
C	-6.576137	-2.888387	0.377898
O	5.629800	1.652654	-0.758707
C	6.636792	1.321106	-1.716209
H	-3.523371	-5.758704	0.491858
H	-1.766222	-5.611120	0.263246
H	-2.868252	-5.687796	-1.126323
H	-7.328260	-3.610336	0.705655
H	-7.022359	-2.297090	-0.431750
H	-6.321676	-2.210918	1.198347
H	-5.554318	-0.731335	-0.326273
H	-1.747573	-0.782812	-0.046234
H	-0.201656	-4.290761	-0.062319
H	-6.099936	1.690055	0.181929
H	-6.002122	1.014591	-2.244909
H	-4.677299	2.164467	-2.501239
H	-6.296367	2.757253	-2.073706
H	-4.620888	5.000770	3.058182
H	-4.364077	5.611960	1.416881
H	-3.126042	4.614049	2.200766
H	-4.666530	2.637353	2.161232
H	-5.962624	3.638498	1.517078
H	-4.647332	4.008010	-0.577805
H	-2.152720	4.618666	-0.054938
H	0.081362	5.919261	0.770513
H	0.084104	5.863627	-0.993924
H	1.618169	5.861920	-0.108614
H	4.016163	1.395151	1.074918
H	-0.848275	1.085648	0.025372
H	2.725805	-1.950980	2.409191
H	3.873712	-0.685701	1.981727
H	3.734032	-1.495512	-0.443710
H	1.778152	-4.292271	-1.711119
H	3.467056	-3.787444	-1.485367
H	2.294715	-2.662999	-2.197852
H	2.246154	-3.696726	0.693303
H	7.525574	1.876194	-1.416183
H	6.324642	1.615167	-2.722023
H	6.830213	0.244493	-1.689305
H	4.958432	-2.809234	2.874746
H	4.391178	-3.676457	1.472203
C	5.900318	-2.250273	1.081671
O	6.845838	-3.206147	1.116923
O	6.069447	-1.190507	0.520291
H	7.622557	-2.870562	0.640322