Supporting information

The Photochemical Reactivity and Theoretical Study of Triplet Furano- and Pyrano- 1,4-Naphthoquionones towards Indole, Phenols and Amino Acid Derivatives

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Additional Data

Figure S1. Transient absorption spectrum recorded upon excitation (355 nm) of **1b, 1e, 2b e 2e** in acetonitrile.

Figure S2. Transient absorption spectrum recorded upon excitation (355 nm) of **2a** in 2-propanol. Inset: Decay at 370 nm.

Figure S3. Quenching plots of **1a** by phenol, 4-methoxyphenol and 4-cyanophenol in acetonitrile. λ_{mon} = 450 nm.
Figure S4. Quenching plots of **2e** by phenol, 4-methoxyphenol and 4-cyanophenol in acetonitrile. λ_{mon} = 450 nm.
Figure S5. Quenching plots of **1e** by NATrpME in acetonitrile. λ_{mon} = 450 nm.
Figure S6. Quenching plots of **1e** by NATyrME in acetonitrile. λ_{mon} = 450 nm.
Figure S7. Quenching plots of **2b** by indole in acetonitrile. λ_{mon} = 450 nm.
Figure S8. LFP spectra observed for **1a** in 0.68 mmolL^{-1} of indole in ACN (λ_{exc}= 355nm).
Figure S9. LFP spectra observed for **2a** in 0.68 mmol.L^{-1} of indole in ACN (λ_{exc}= 355nm).
Figure S10. LFP spectra observed for **1a** in 0.51 mmol.L^{-1} of phenol in ACN (λ_{exc}= 355nm).
Figure S11. LFP spectra observed for **2a** in 0.51 mmol.L^{-1} of phenol in ACN (λ_{exc}= 355nm).
Theoretical Calculations: Atomic Coordinates and Thermodynamics

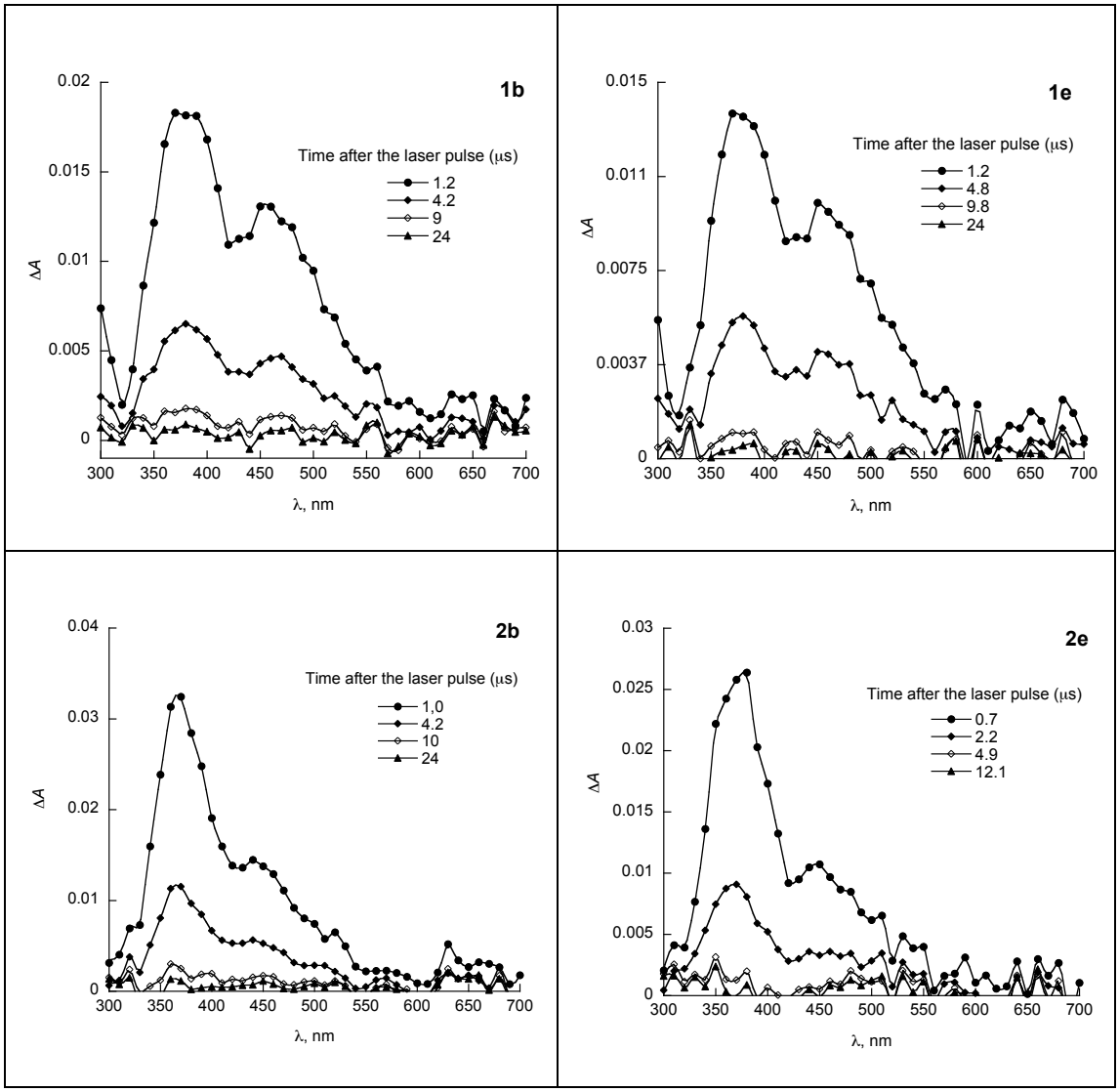


Figure S1. Transient absorption spectrum recorded upon excitation (355 nm) of **1b, 1e, 2b e 2e** in acetonitrile.

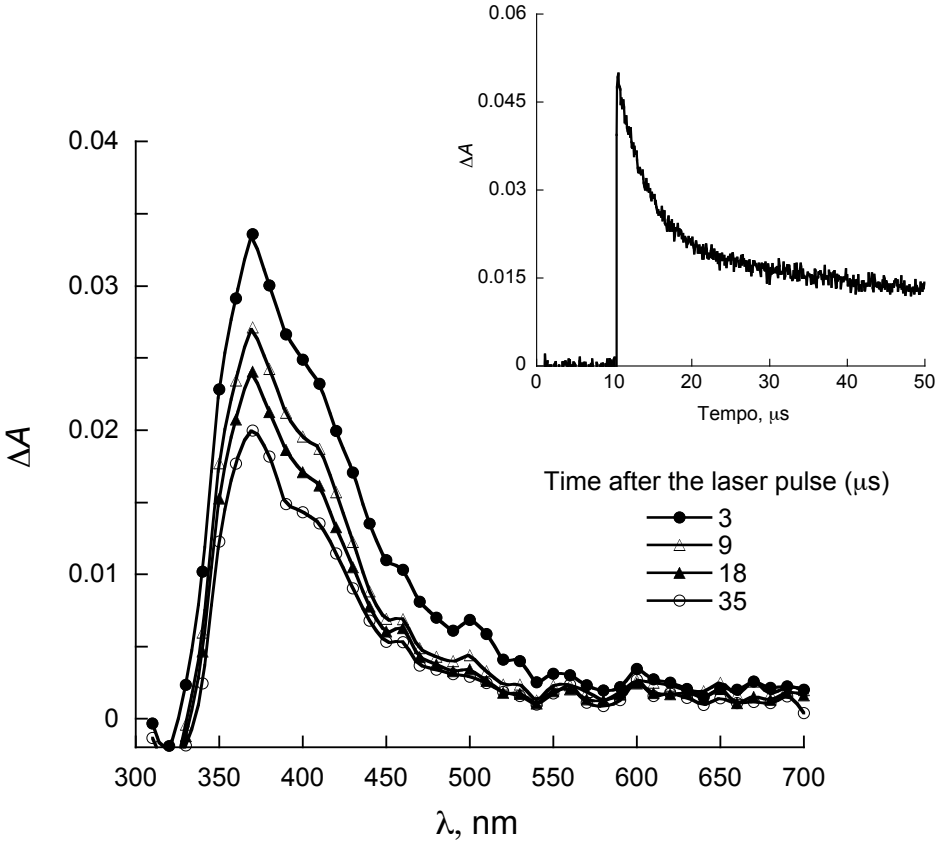


Figure S2. Transient absorption spectrum recorded upon excitation (355 nm) of **2a** in 2-propanol. Inset: Decay at 370 nm.

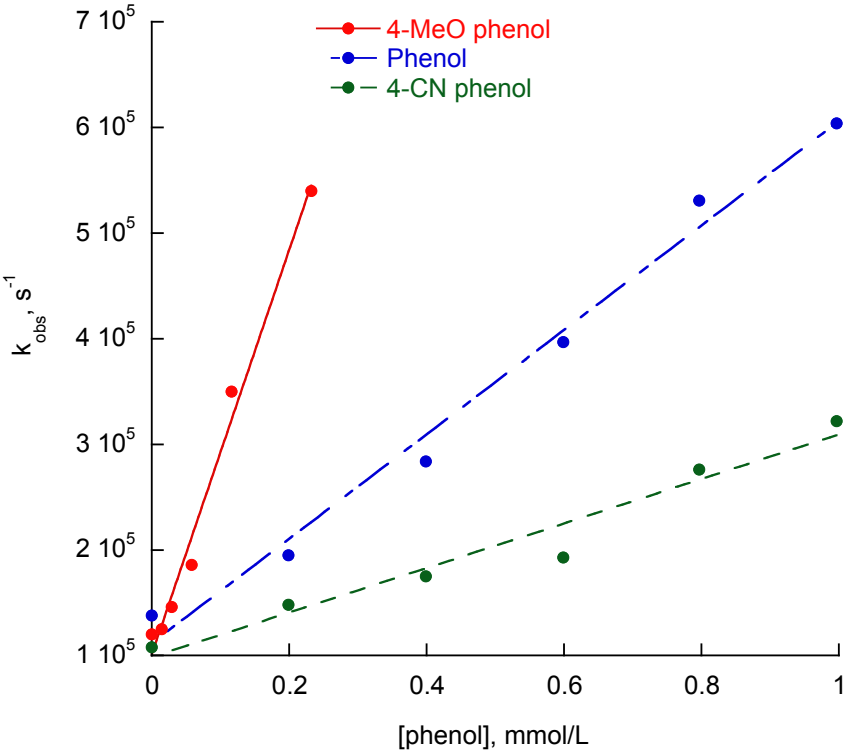


Figure S3. Quenching plots of **1a** by phenol, 4-methoxyphenol and 4-cyanophenol in acetonitrile. λ_{mon} = 450 nm.

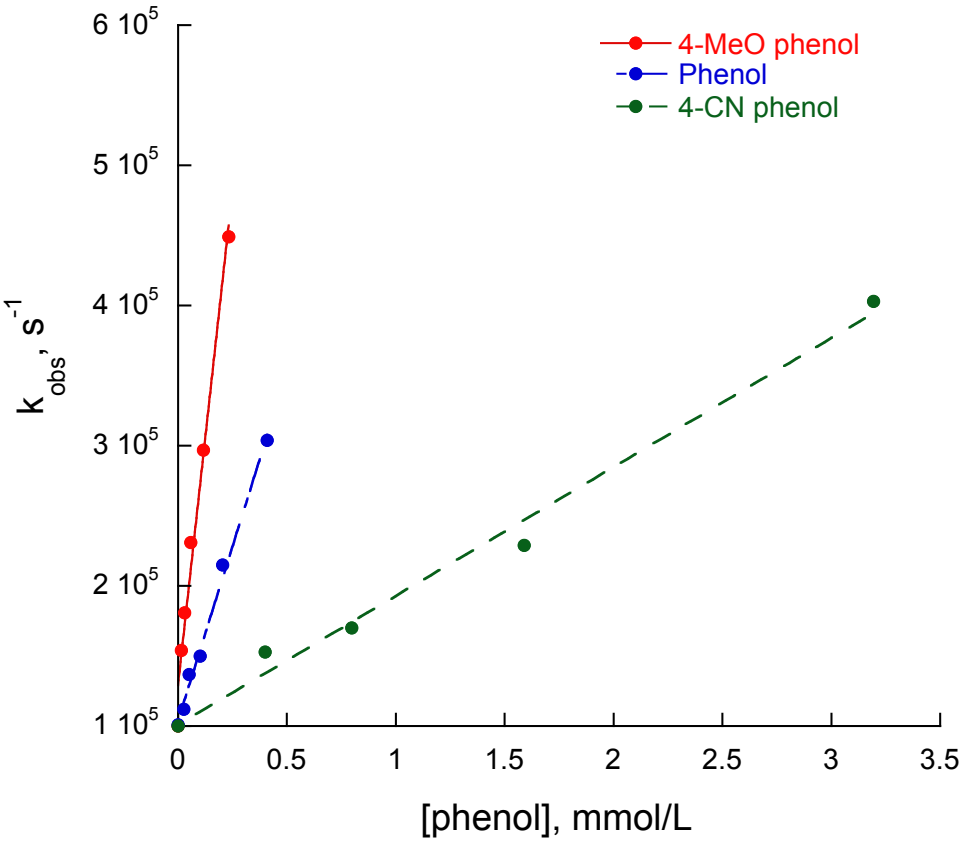


Figure S4. Quenching plots of **2e** by phenol, 4-methoxyphenol and 4-cyanophenol in acetonitrile. λ_{mon} = 450 nm.

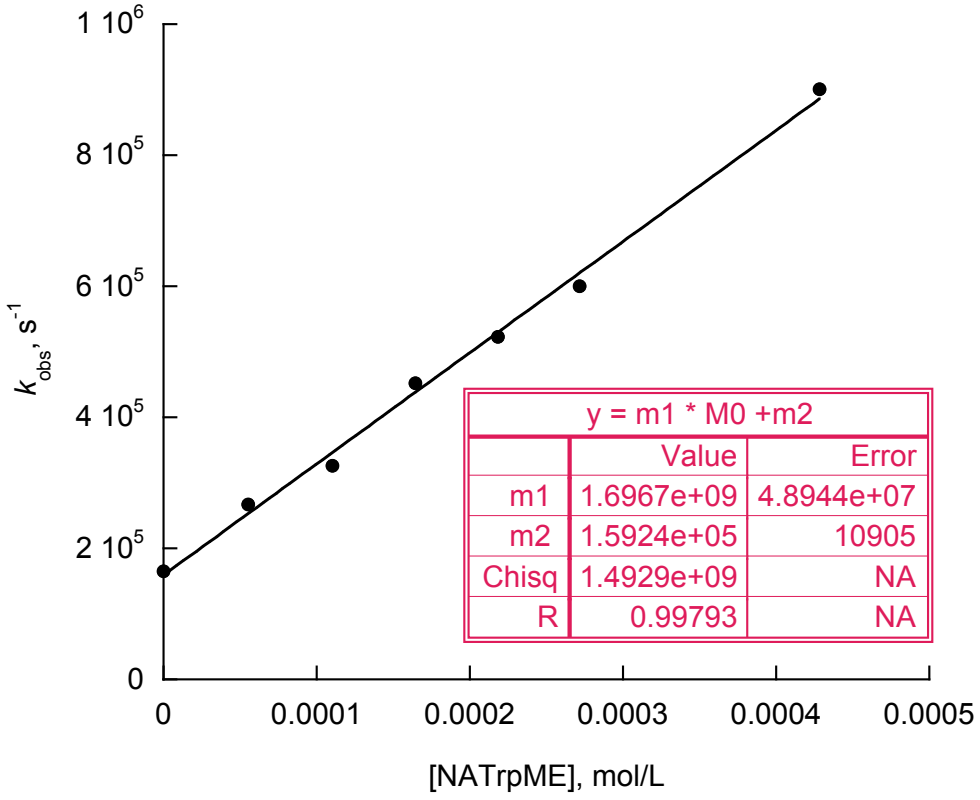


Figure S5. Quenching plots of **1e** by NATrpME in acetonitrile. λ_{mon} = 450 nm.

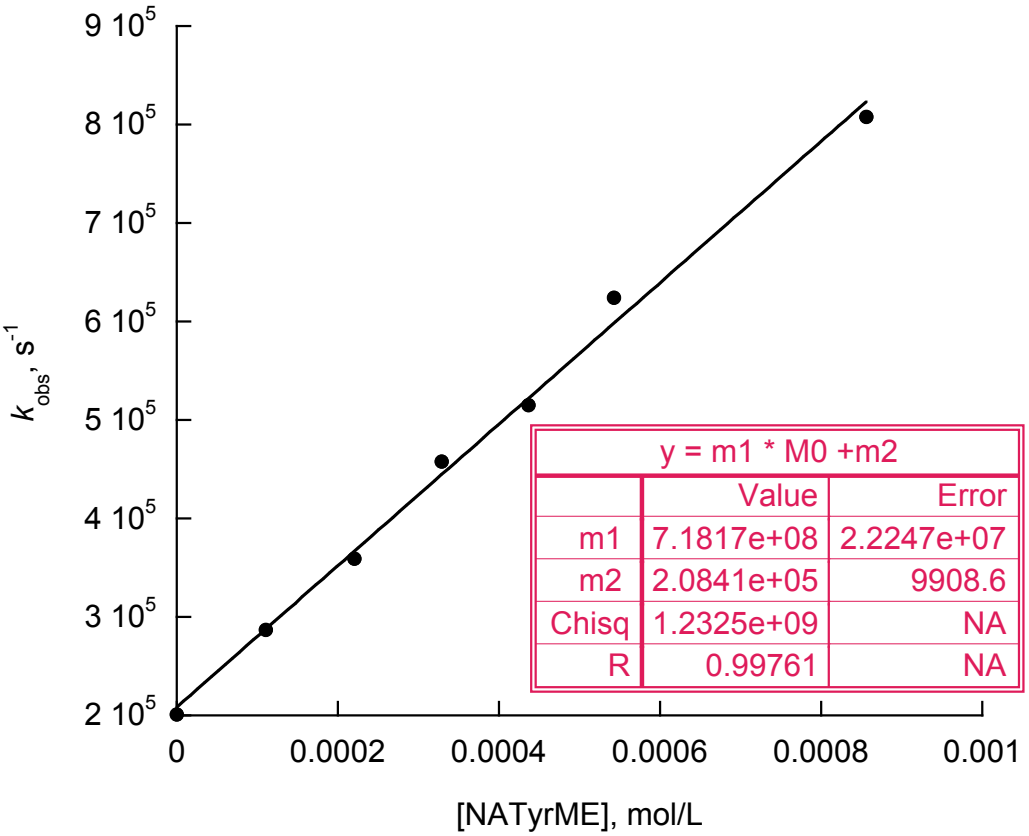


Figure S6. Quenching plots of **1e** by NATyrME in acetonitrile. λ_{mon} = 450 nm.

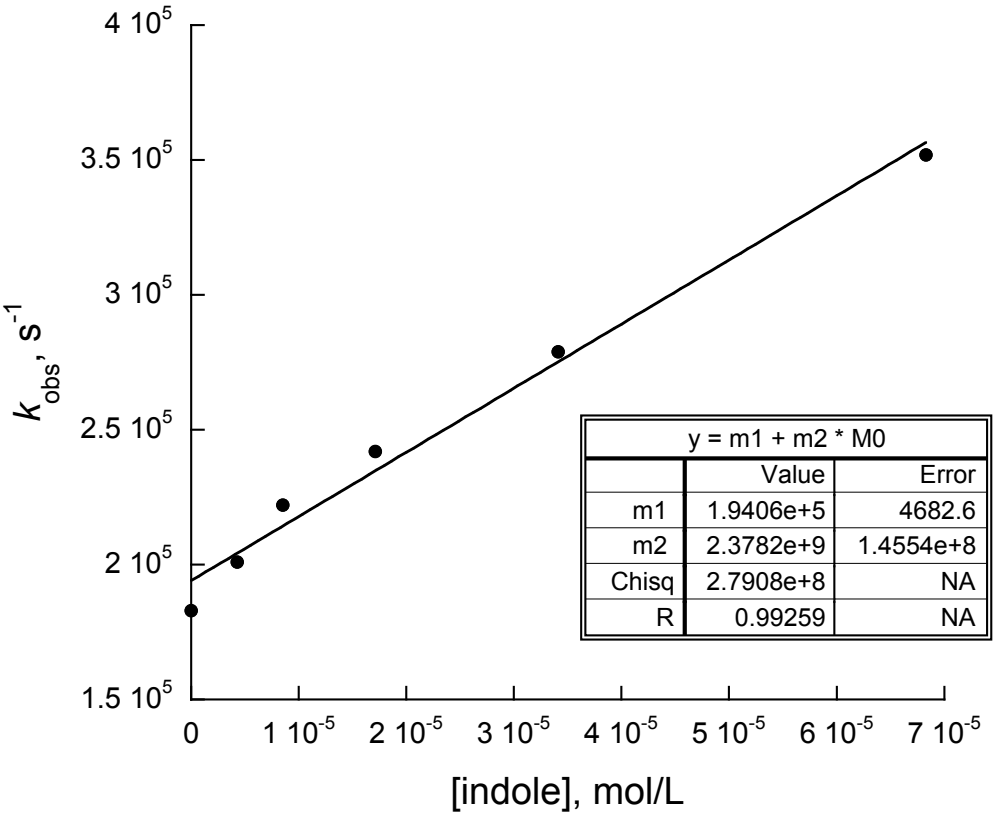


Figure S7. Quenching plots of **2b** by indole in acetonitrile. λ_{mon} = 450 nm.

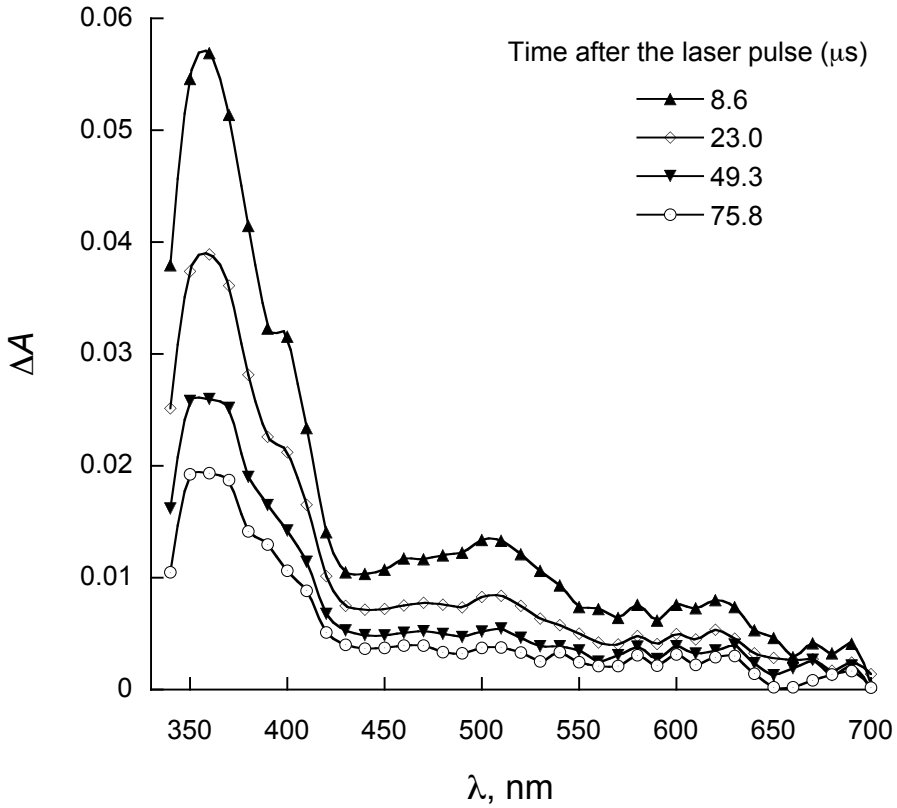


Figure S8. LFP spectra observed for **1a** in 0.68 mmolL^{-1} of indole in ACN (λ_{exc}= 355nm).

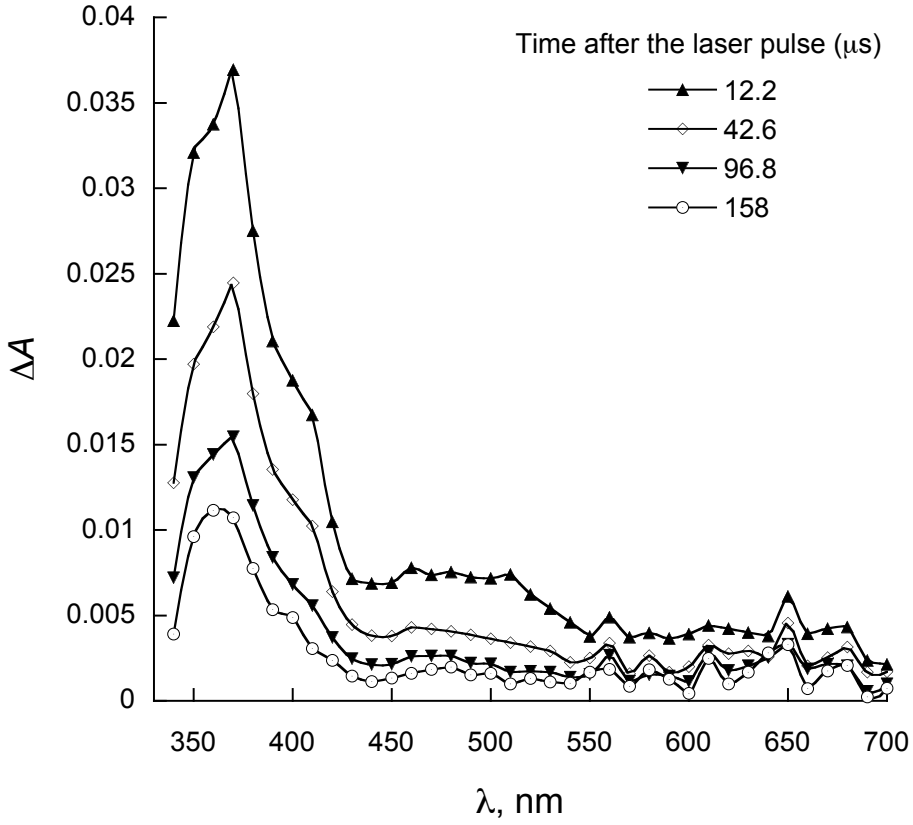


Figure S9. LFP spectra observed for **2a** in 0.68 mmol.L^{-1} of indole in ACN (λ_{exc}= 355nm).

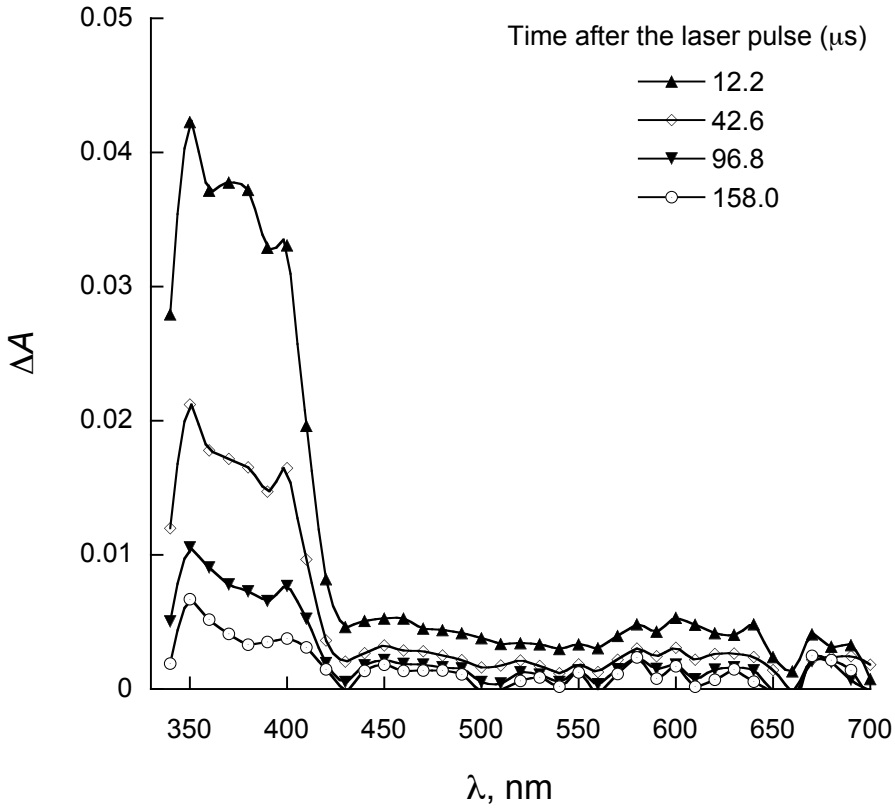


Figure S10. LFP spectra observed for **1a** in 0.51 mmol.L^{-1} of phenol in ACN (λ_{exc}= 355nm).

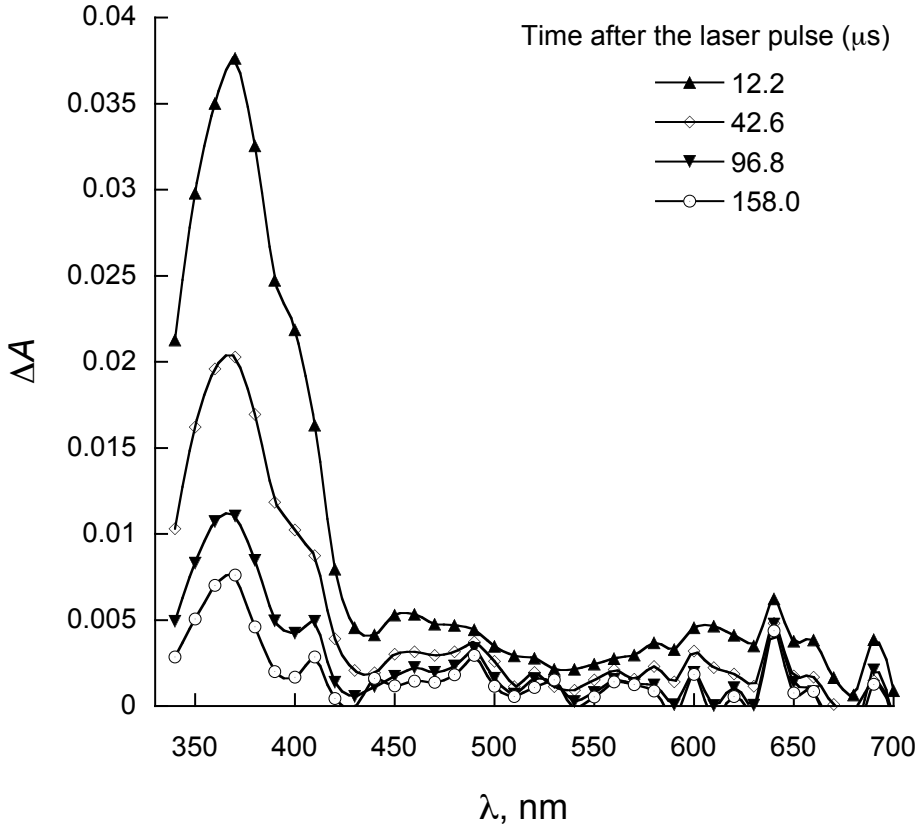


Figure S11. LFP spectra observed for **2a** in 0.51 mmol.L^{-1} of phenol in ACN (λ_{exc}= 355nm).

Theoretical Calculations
Atomic coordinates of optimized NQF-Phenol structures
[(u)b3lyp/6-31g(d) scrf=(iefpcm,solvent=acetonitrile)]

Ground state S_0 complexes

ACN-NQF-PhOH-S0-01-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.805706	1.722327	-0.688147
2	6	0	0.192990	2.000154	-0.369202
3	6	0	2.767978	2.707315	0.457485
4	6	0	1.167875	1.008877	-0.208971
5	6	0	0.503107	3.337703	-0.118385
6	6	0	1.788896	3.691213	0.293938
7	6	0	2.471660	1.368101	0.210716
8	1	0	-0.258953	4.100447	-0.245033
9	1	0	2.031386	4.731558	0.489041
10	1	0	3.771711	2.965571	0.778063
11	6	0	0.825296	-0.410874	-0.478709
12	6	0	1.926680	-1.378630	-0.268063
13	6	0	3.173752	-1.039534	0.131220
14	6	0	3.551192	0.337512	0.400063
15	8	0	4.686387	0.651527	0.762938
16	8	0	1.718528	-2.684416	-0.480801
17	6	0	2.986779	-3.378359	-0.186188
18	1	0	3.264465	-3.918481	-1.092686
19	1	0	2.772896	-4.092149	0.611149
20	6	0	4.012709	-2.287877	0.222952
21	1	0	4.871684	-2.252670	-0.455912
22	1	0	4.402995	-2.446567	1.233919
23	8	0	-0.280611	-0.803799	-0.853873
24	1	0	-1.931379	-0.091692	-1.225516
25	8	0	-2.784000	0.348620	-1.432137
26	6	0	-3.740068	-0.032674	-0.534729
27	6	0	-5.787342	-0.744250	1.246564
28	6	0	-5.016169	0.531504	-0.668247
29	6	0	-3.488893	-0.954340	0.491680
30	6	0	-4.513565	-1.303385	1.373756
31	6	0	-6.029783	0.173871	0.219689
32	1	0	-5.194850	1.243684	-1.468711
33	1	0	-2.499795	-1.393369	0.591712
34	1	0	-4.309423	-2.019195	2.166013
35	1	0	-7.016109	0.616863	0.107507
36	1	0	-6.579916	-1.019748	1.936183

ACN-NQF-PhOH-S0-01-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.694109	-2.825360	-0.784919
2	6	0	-1.682015	-2.490168	-0.487198
3	6	0	-4.213191	-1.583548	0.280575
4	6	0	-1.894529	-1.126479	-0.260628
5	6	0	-2.729751	-3.398572	-0.331107
6	6	0	-3.993513	-2.945225	0.052859
7	6	0	-3.174917	-0.666341	0.127220
8	1	0	-2.559517	-4.455978	-0.508417
9	1	0	-4.809905	-3.650631	0.175505
10	1	0	-5.189923	-1.217595	0.579001
11	6	0	-0.765617	-0.179052	-0.429290
12	6	0	-1.088540	1.241709	-0.173379
13	6	0	-2.309816	1.688838	0.197801
14	6	0	-3.441187	0.792701	0.377974
15	8	0	-4.555008	1.197589	0.715115
16	8	0	-0.139336	2.177420	-0.302702
17	6	0	-0.762605	3.474740	0.024489
18	1	0	-0.634716	4.111208	-0.852400
19	1	0	-0.197605	3.888828	0.861071
20	6	0	-2.248781	3.185106	0.367123
21	1	0	-2.937087	3.701300	-0.310792
22	1	0	-2.504236	3.492151	1.386982
23	8	0	0.367924	-0.535106	-0.757989
24	1	0	1.917744	0.496352	-0.818173
25	8	0	2.785335	0.947765	-0.908197
26	6	0	3.768600	0.210473	-0.323516
27	6	0	5.886694	-1.213412	0.851776
28	6	0	5.069217	0.736839	-0.338993
29	6	0	3.532020	-1.033474	0.281654
30	6	0	4.590573	-1.734097	0.863590
31	6	0	6.116238	0.026235	0.245721
32	1	0	5.238699	1.700512	-0.810977
33	1	0	2.526559	-1.444659	0.289974
34	1	0	4.395084	-2.696901	1.329345
35	1	0	7.119143	0.445510	0.227369
36	1	0	6.705267	-1.763721	1.306593

ACN-NQF-PhOH-S0-02-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	-3.756479	2.971515	0.783030
2	6	0	-2.753896	2.712464	0.458962
3	6	0	-0.185365	1.994663	-0.376191
4	6	0	-2.454846	1.371288	0.209405
5	6	0	-1.776190	3.694892	0.292709
6	6	0	-0.494104	3.334509	-0.123727
7	6	0	-1.155068	1.003268	-0.215040
8	1	0	-2.015306	4.735729	0.488156
9	1	0	0.270164	4.094826	-0.253389
10	1	0	0.812460	1.718405	-0.698129
11	6	0	-3.525221	0.352095	0.401809
12	6	0	-3.108843	-1.045800	0.114445
13	6	0	-1.866280	-1.400571	-0.291501
14	6	0	-0.812896	-0.430988	-0.489661
15	8	0	-3.981082	-2.047335	0.250822
16	6	0	-3.273357	-3.294736	-0.102091
17	1	0	-3.832631	-3.745969	-0.923028
18	1	0	-3.328970	-3.940832	0.775418
19	6	0	-1.823928	-2.895346	-0.485577
20	1	0	-1.581219	-3.166946	-1.518420
21	1	0	-1.080286	-3.372470	0.161448
22	8	0	-4.662580	0.620005	0.766575
23	8	0	0.314786	-0.786252	-0.870208
24	1	0	1.920253	-0.068748	-1.229198
25	8	0	2.784450	0.352403	-1.441097
26	6	0	3.730776	-0.031428	-0.536378
27	6	0	5.761520	-0.752892	1.261808
28	6	0	5.019100	0.503417	-0.677147
29	6	0	3.459952	-0.929200	0.506801
30	6	0	4.476109	-1.283093	1.396638
31	6	0	6.024017	0.141231	0.218800
32	1	0	5.213795	1.197114	-1.490083
33	1	0	2.461710	-1.345334	0.611691
34	1	0	4.256267	-1.980106	2.201468
35	1	0	7.019460	0.561717	0.100204
36	1	0	6.547320	-1.032130	1.957697

ACN-NQF-PhOH-S0-02-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.108714	-1.294399	-0.699455
2	6	0	4.139557	-1.636249	-0.351319
3	6	0	1.625981	-2.469442	0.544162
4	6	0	3.124776	-0.696070	-0.157030

5	6	0	3.902246	-2.988733	-0.099508
6	6	0	2.646551	-3.403798	0.348068
7	6	0	1.852204	-1.115120	0.295440
8	1	0	4.694843	-3.714814	-0.252123
9	1	0	2.459174	-4.454994	0.545317
10	1	0	0.646867	-2.780311	0.892176
11	6	0	3.406200	0.739534	-0.433364
12	6	0	2.256728	1.654375	-0.192918
13	6	0	1.035756	1.255908	0.241908
14	6	0	0.741617	-0.132483	0.513439
15	8	0	2.395931	2.964056	-0.404822
16	6	0	1.092020	3.595355	-0.119709
17	1	0	0.757229	4.047609	-1.055026
18	1	0	1.280178	4.377419	0.616742
19	6	0	0.152337	2.471397	0.388296
20	1	0	-0.763630	2.396764	-0.205362
21	1	0	-0.149753	2.627556	1.429859
22	8	0	4.486534	1.160478	-0.825449
23	8	0	-0.370609	-0.519866	0.911057
24	1	0	-1.912267	0.390796	0.967355
25	8	0	-2.760985	0.892889	0.981710
26	6	0	-3.737447	0.190059	0.343768
27	6	0	-5.832415	-1.168026	-0.943699
28	6	0	-5.010358	0.773480	0.258465
29	6	0	-3.516066	-1.076802	-0.217997
30	6	0	-4.563098	-1.744881	-0.856009
31	6	0	-6.046390	0.094816	-0.381613
32	1	0	-5.168085	1.754546	0.697517
33	1	0	-2.530371	-1.528708	-0.149681
34	1	0	-4.380154	-2.726106	-1.287090
35	1	0	-7.028425	0.557447	-0.440974
36	1	0	-6.642458	-1.693179	-1.441496

Relaxed T_1 complexes

ACN-NQF-PhOH-T1-01-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.818958	1.691507	-0.704887
2	6	0	0.177423	1.972123	-0.382865
3	6	0	2.744625	2.696743	0.451079
4	6	0	1.150917	0.964643	-0.220550
5	6	0	0.480344	3.301784	-0.135918
6	6	0	1.771487	3.669372	0.283506
7	6	0	2.461725	1.341190	0.207008

8	1	0	-0.283850	4.062401	-0.266952
9	1	0	2.004735	4.712471	0.475734
10	1	0	3.747051	2.956994	0.774418
11	6	0	0.780543	-0.436560	-0.495687
12	6	0	1.847520	-1.363060	-0.289931
13	6	0	3.185141	-1.004666	0.142302
14	6	0	3.547278	0.354503	0.407626
15	8	0	4.705117	0.659956	0.781405
16	8	0	1.730876	-2.667143	-0.477906
17	6	0	3.003831	-3.344186	-0.185135
18	1	0	3.280851	-3.872771	-1.098401
19	1	0	2.786161	-4.066371	0.603161
20	6	0	3.996750	-2.244507	0.229763
21	1	0	4.869369	-2.197529	-0.434706
22	1	0	4.389061	-2.395837	1.243766
23	8	0	-0.359685	-0.828414	-0.879935
24	1	0	-1.900106	-0.091713	-1.236336
25	8	0	-2.771337	0.321952	-1.457272
26	6	0	-3.712311	-0.039366	-0.540712
27	6	0	-5.734615	-0.718439	1.286106
28	6	0	-5.005242	0.482921	-0.692305
29	6	0	-3.433899	-0.903871	0.529264
30	6	0	-4.445340	-1.236584	1.432305
31	6	0	-6.005400	0.142121	0.217273
32	1	0	-5.206925	1.150695	-1.525127
33	1	0	-2.432410	-1.309736	0.641156
34	1	0	-4.219038	-1.907722	2.257250
35	1	0	-7.003737	0.553071	0.089161
36	1	0	-6.516642	-0.981231	1.992654

ACN-NQF-PhOH-T1-01-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.676828	-2.790807	-0.874552
2	6	0	-1.654660	-2.465371	-0.536533
3	6	0	-4.162203	-1.587040	0.333831
4	6	0	-1.851717	-1.091371	-0.292352
5	6	0	-2.683516	-3.374613	-0.350201
6	6	0	-3.946094	-2.934323	0.088103
7	6	0	-3.133177	-0.646224	0.151505
8	1	0	-2.514787	-4.430104	-0.542915
9	1	0	-4.750198	-3.649660	0.233421
10	1	0	-5.128346	-1.227208	0.671933
11	6	0	-0.719304	-0.172792	-0.506490
12	6	0	-1.028197	1.193091	-0.233108

13	6	0	-2.321946	1.671099	0.220097
14	6	0	-3.422349	0.778906	0.430327
15	8	0	-4.536991	1.199244	0.822031
16	8	0	-0.162762	2.184285	-0.364429
17	6	0	-0.788607	3.465518	-0.000528
18	1	0	-0.696872	4.105106	-0.879524
19	1	0	-0.187170	3.872983	0.813358
20	6	0	-2.240802	3.143388	0.393007
21	1	0	-2.970315	3.661074	-0.243345
22	1	0	-2.468287	3.438031	1.425760
23	8	0	0.420759	-0.559545	-0.899425
24	1	0	1.883741	0.409279	-0.927704
25	8	0	2.746324	0.893467	-0.977616
26	6	0	3.721356	0.194083	-0.341669
27	6	0	5.822945	-1.161077	0.945426
28	6	0	5.010488	0.749672	-0.311567
29	6	0	3.489702	-1.045626	0.276949
30	6	0	4.539065	-1.711309	0.913331
31	6	0	6.048499	0.073637	0.327812
32	1	0	5.178135	1.708857	-0.793520
33	1	0	2.492700	-1.476053	0.251096
34	1	0	4.346602	-2.670515	1.388058
35	1	0	7.041630	0.516002	0.342985
36	1	0	6.634464	-1.684472	1.442825

ACN-NQF-PhOH-T1-02-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.768262	2.925951	0.784958
2	6	0	-2.764889	2.677408	0.456020
3	6	0	-0.192178	1.987456	-0.392305
4	6	0	-2.470809	1.324071	0.206996
5	6	0	-1.802571	3.659845	0.286383
6	6	0	-0.507195	3.312358	-0.140004
7	6	0	-1.155483	0.970367	-0.228188
8	1	0	-2.047650	4.699579	0.483159
9	1	0	0.246465	4.083101	-0.271227
10	1	0	0.805704	1.716792	-0.718953
11	6	0	-3.555437	0.335556	0.415711
12	6	0	-3.150816	-1.007452	0.136557
13	6	0	-1.824062	-1.388643	-0.307618
14	6	0	-0.784047	-0.426800	-0.506982
15	8	0	-3.944852	-2.062458	0.252817
16	6	0	-3.223873	-3.289755	-0.111803
17	1	0	-3.784818	-3.738268	-0.933223

18	1	0	-3.272500	-3.941354	0.762037
19	6	0	-1.796196	-2.860382	-0.491984
20	1	0	-1.538636	-3.127124	-1.525471
21	1	0	-1.033395	-3.327503	0.144678
22	8	0	-4.711814	0.635894	0.798562
23	8	0	0.354841	-0.810223	-0.899084
24	1	0	1.921591	-0.065117	-1.241157
25	8	0	2.790087	0.354881	-1.450170
26	6	0	3.728471	-0.020463	-0.535385
27	6	0	5.744777	-0.726561	1.286733
28	6	0	5.019463	0.510145	-0.671312
29	6	0	3.448580	-0.906650	0.515874
30	6	0	4.457192	-1.252813	1.417117
31	6	0	6.016812	0.155795	0.236147
32	1	0	5.221974	1.194746	-1.490089
33	1	0	2.448508	-1.319255	0.616399
34	1	0	4.229861	-1.940698	2.227789
35	1	0	7.013963	0.573210	0.120687
36	1	0	6.524663	-0.999702	1.991677

ACN-NQF-PhOH-T1-02-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.034905	-1.210401	-0.857544
2	6	0	4.099099	-1.571468	-0.444338
3	6	0	1.669543	-2.457232	0.618992
4	6	0	3.081587	-0.631519	-0.196366
5	6	0	3.909370	-2.916228	-0.167860
6	6	0	2.686258	-3.363125	0.367817
7	6	0	1.840918	-1.084932	0.345662
8	1	0	4.706128	-3.627816	-0.364435
9	1	0	2.540844	-4.417474	0.583427
10	1	0	0.720854	-2.783350	1.031664
11	6	0	3.353381	0.788535	-0.518730
12	6	0	2.250449	1.651114	-0.224125
13	6	0	0.986665	1.215060	0.340883
14	6	0	0.729595	-0.163041	0.628821
15	8	0	2.260003	2.959588	-0.439491
16	6	0	0.965892	3.547327	-0.071529
17	1	0	0.538998	3.945410	-0.994442
18	1	0	1.186208	4.367875	0.612067
19	6	0	0.134434	2.412437	0.548158
20	1	0	-0.857274	2.298903	0.092601
21	1	0	-0.046138	2.575843	1.620560
22	8	0	4.433410	1.202100	-1.004558

23	8	0	-0.377644	-0.551641	1.101853
24	1	0	-1.892939	0.337109	1.065440
25	8	0	-2.724368	0.869309	0.998471
26	6	0	-3.683330	0.170083	0.330249
27	6	0	-5.738645	-1.181059	-1.023957
28	6	0	-4.932553	0.782857	0.151754
29	6	0	-3.464402	-1.121397	-0.173445
30	6	0	-4.492246	-1.786515	-0.844320
31	6	0	-5.949375	0.107035	-0.521095
32	1	0	-5.087865	1.782906	0.546524
33	1	0	-2.494918	-1.592054	-0.035026
34	1	0	-4.312543	-2.787048	-1.229825
35	1	0	-6.913690	0.591399	-0.652724
36	1	0	-6.533627	-1.703743	-1.547905

Optimized T1-TS for H-abstraction

ACN-NQF-PhOH-T1-TS-01-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.016401	2.456734	-1.307162
2	6	0	0.928263	2.354248	-0.729074
3	6	0	3.304438	2.091726	0.715794
4	6	0	1.396715	1.058942	-0.412363
5	6	0	1.624014	3.483173	-0.325611
6	6	0	2.818050	3.354768	0.406159
7	6	0	2.619577	0.932874	0.317043
8	1	0	1.246988	4.469704	-0.580871
9	1	0	3.361109	4.241277	0.721552
10	1	0	4.228816	1.967613	1.271053
11	6	0	0.642707	-0.116398	-0.839793
12	6	0	1.238972	-1.365833	-0.511919
13	6	0	2.436630	-1.514051	0.194516
14	6	0	3.192815	-0.392216	0.657187
15	8	0	4.265097	-0.519941	1.301006
16	8	0	0.666857	-2.541232	-0.843838
17	6	0	1.503322	-3.629017	-0.331670
18	1	0	1.770865	-4.251317	-1.188543
19	1	0	0.879506	-4.211337	0.350693
20	6	0	2.721899	-2.976372	0.360248
21	1	0	3.668243	-3.264773	-0.114206
22	1	0	2.799941	-3.262789	1.416160
23	8	0	-0.480630	-0.067156	-1.477400
24	1	0	-1.507588	0.778716	-1.072907
25	8	0	-2.346910	1.363454	-0.742378

26	6	0	-3.292783	0.644420	-0.186474
27	6	0	-5.386381	-0.796451	0.985680
28	6	0	-4.435566	1.328364	0.328471
29	6	0	-3.216228	-0.780006	-0.092030
30	6	0	-4.258456	-1.477329	0.486992
31	6	0	-5.464398	0.608362	0.900763
32	1	0	-4.466446	2.409666	0.246549
33	1	0	-2.333216	-1.278860	-0.477192
34	1	0	-4.207105	-2.559022	0.562207
35	1	0	-6.337428	1.123816	1.288273
36	1	0	-6.196938	-1.355669	1.441767

ACN-NQF-PhOH-T1-TS-01-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.738049	-2.806505	-1.005917
2	6	0	-1.678698	-2.444235	-0.604543
3	6	0	-4.087891	-1.476458	0.429058
4	6	0	-1.805344	-1.064220	-0.336160
5	6	0	-2.730271	-3.314535	-0.363752
6	6	0	-3.944259	-2.829838	0.156937
7	6	0	-3.037342	-0.573943	0.192175
8	1	0	-2.616276	-4.373767	-0.577707
9	1	0	-4.766882	-3.514170	0.345105
10	1	0	-5.015122	-1.081123	0.831767
11	6	0	-0.676464	-0.173949	-0.596687
12	6	0	-0.917168	1.196415	-0.303648
13	6	0	-2.111833	1.700748	0.224242
14	6	0	-3.238173	0.863259	0.498966
15	8	0	-4.315924	1.313329	0.964905
16	8	0	0.011155	2.150762	-0.523242
17	6	0	-0.505819	3.426910	-0.022542
18	1	0	-0.381531	4.152697	-0.828111
19	1	0	0.127862	3.714985	0.820440
20	6	0	-1.976355	3.185023	0.384718
21	1	0	-2.675357	3.725812	-0.266725
22	1	0	-2.181748	3.514585	1.409697
23	8	0	0.445783	-0.613966	-1.055989
24	1	0	1.610944	0.209963	-1.026189
25	8	0	2.539791	0.734149	-1.004501
26	6	0	3.480604	0.099653	-0.343972
27	6	0	5.567482	-1.172825	1.022796
28	6	0	4.766219	0.712903	-0.262995
29	6	0	3.259926	-1.164109	0.282972
30	6	0	4.300178	-1.782124	0.950854

31	6	0	5.789499	0.076531	0.411695
32	1	0	4.907413	1.674207	-0.745788
33	1	0	2.274325	-1.612325	0.218887
34	1	0	4.137914	-2.743591	1.428186
35	1	0	6.769352	0.539730	0.471829
36	1	0	6.374965	-1.665936	1.554466

ACN-NQF-PhOH-T1-TS-02-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.278548	2.242398	-0.971927
2	6	0	-3.289315	2.269680	-0.526377
3	6	0	-0.750937	2.283554	0.637714
4	6	0	-2.666594	1.041302	-0.237113
5	6	0	-2.663304	3.474202	-0.245413
6	6	0	-1.387128	3.480003	0.347462
7	6	0	-1.359905	1.043585	0.345331
8	1	0	-3.160228	4.412868	-0.474560
9	1	0	-0.900981	4.422587	0.582779
10	1	0	0.225324	2.293993	1.108665
11	6	0	-3.401249	-0.204558	-0.535903
12	6	0	-2.678650	-1.390632	-0.170755
13	6	0	-1.389137	-1.400207	0.391330
14	6	0	-0.668415	-0.214077	0.648504
15	8	0	-3.181897	-2.624287	-0.351700
16	6	0	-2.216216	-3.608829	0.140288
17	1	0	-2.020856	-4.297069	-0.684630
18	1	0	-2.707431	-4.153040	0.950546
19	6	0	-0.969051	-2.823548	0.602233
20	1	0	-0.080978	-3.076327	0.009252
21	1	0	-0.716215	-3.027870	1.649381
22	8	0	-4.549123	-0.229840	-1.050409
23	8	0	0.524857	-0.274415	1.136390
24	1	0	1.592470	0.609414	0.802375
25	8	0	2.426011	1.212092	0.551628
26	6	0	3.465386	0.524142	0.127520
27	6	0	5.746534	-0.841666	-0.745295
28	6	0	4.626684	1.249155	-0.267733
29	6	0	3.463021	-0.900240	0.062861
30	6	0	4.597877	-1.562491	-0.366615
31	6	0	5.749872	0.565380	-0.691800
32	1	0	4.600422	2.332397	-0.213551
33	1	0	2.561097	-1.431456	0.348060
34	1	0	4.601587	-2.646845	-0.418735
35	1	0	6.638835	1.114232	-0.986397

36	1	0	6.629883	-1.372199	-1.085967

ACN-NQF-PhOH-T1-TS-02-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.018806	-1.264649	-0.717613
2	6	0	4.054679	-1.614948	-0.363153
3	6	0	1.553890	-2.465344	0.548785
4	6	0	3.040360	-0.658929	-0.163626
5	6	0	3.828228	-2.959377	-0.113322
6	6	0	2.568099	-3.387598	0.346638
7	6	0	1.762423	-1.092386	0.301986
8	1	0	4.622746	-3.683536	-0.271400
9	1	0	2.391018	-4.441361	0.543145
10	1	0	0.578727	-2.781409	0.903748
11	6	0	3.337994	0.759068	-0.446433
12	6	0	2.227302	1.633604	-0.192169
13	6	0	0.963547	1.219978	0.276720
14	6	0	0.669150	-0.140639	0.522901
15	8	0	2.305388	2.961475	-0.384850
16	6	0	1.020619	3.569782	-0.042348
17	1	0	0.657199	4.068466	-0.944062
18	1	0	1.221835	4.321328	0.724089
19	6	0	0.098951	2.431331	0.441737
20	1	0	-0.829091	2.360956	-0.143415
21	1	0	-0.214542	2.569994	1.484460
22	8	0	4.450921	1.167789	-0.867174
23	8	0	-0.485436	-0.551471	0.925337
24	1	0	-1.644025	0.271895	0.880730
25	8	0	-2.545764	0.837471	0.836610
26	6	0	-3.544946	0.183343	0.277492
27	6	0	-5.739505	-1.125704	-0.864996
28	6	0	-4.807768	0.836542	0.200425
29	6	0	-3.398107	-1.135997	-0.240688
30	6	0	-4.492043	-1.773303	-0.797725
31	6	0	-5.886369	0.180992	-0.363056
32	1	0	-4.892457	1.842132	0.598986
33	1	0	-2.424583	-1.612113	-0.190039
34	1	0	-4.385170	-2.778573	-1.193524
35	1	0	-6.851233	0.675318	-0.418741
36	1	0	-6.589112	-1.633039	-1.310750

Relaxed Triplet Radical Pair Products

ACN-NQF-PhOH-T1-01-1-prod

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.813408	1.766559	-0.773609
2	6	0	0.185896	2.003713	-0.425623
3	6	0	2.746019	2.688046	0.458393
4	6	0	1.141181	0.976924	-0.233171
5	6	0	0.508293	3.330460	-0.178995
6	6	0	1.791940	3.680619	0.267024
7	6	0	2.450966	1.340537	0.216819
8	1	0	-0.242221	4.100271	-0.334868
9	1	0	2.038635	4.720850	0.459224
10	1	0	3.747496	2.930244	0.799422
11	6	0	0.840397	-0.413237	-0.479838
12	6	0	1.873961	-1.357082	-0.280603
13	6	0	3.139262	-1.026216	0.146668
14	6	0	3.516132	0.324468	0.435231
15	8	0	4.658200	0.640975	0.842802
16	8	0	1.682688	-2.685625	-0.488812
17	6	0	2.976333	-3.346219	-0.299356
18	1	0	3.299598	-3.708147	-1.279827
19	1	0	2.807083	-4.200834	0.358319
20	6	0	3.945904	-2.290058	0.287167
21	1	0	4.891159	-2.251867	-0.264773
22	1	0	4.194505	-2.494390	1.336321
23	8	0	-0.335347	-0.899019	-0.898716
24	1	0	-1.080262	-0.241756	-0.953629
25	8	0	-2.635720	0.494401	-1.109857
26	6	0	-3.622720	0.074817	-0.432388
27	6	0	-5.841371	-0.829662	1.053895
28	6	0	-4.910261	0.732976	-0.537170
29	6	0	-3.508707	-1.062961	0.459408
30	6	0	-4.600442	-1.493283	1.178307
31	6	0	-5.985225	0.281492	0.193852
32	1	0	-4.984782	1.583529	-1.207120
33	1	0	-2.543602	-1.554019	0.533358
34	1	0	-4.514419	-2.345481	1.845364
35	1	0	-6.948592	0.775628	0.114330
36	1	0	-6.695109	-1.178445	1.626428

ACN-NQF-PhOH-T1-01-2-prod

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.254622	-2.971870	-0.788502
2	6	0	-2.136363	-2.435297	-0.455299
3	6	0	-4.402195	-1.038453	0.404630
4	6	0	-2.054843	-1.038587	-0.256885
5	6	0	-3.326204	-3.111077	-0.227305
6	6	0	-4.466287	-2.413117	0.204517
7	6	0	-3.213594	-0.330603	0.182210
8	1	0	-3.374012	-4.185043	-0.384203
9	1	0	-5.395876	-2.946576	0.381651
10	1	0	-5.271151	-0.479783	0.737616
11	6	0	-0.822497	-0.328535	-0.487001
12	6	0	-0.813503	1.063306	-0.262787
13	6	0	-1.918525	1.769014	0.161119
14	6	0	-3.183932	1.140268	0.404347
15	8	0	-4.197854	1.775341	0.777269
16	8	0	0.297365	1.823413	-0.455280
17	6	0	-0.018162	3.176642	0.010630
18	1	0	0.331890	3.869310	-0.756461
19	1	0	0.550757	3.341324	0.930493
20	6	0	-1.547320	3.226352	0.250219
21	1	0	-2.065553	3.819134	-0.514392
22	1	0	-1.794220	3.667803	1.221401
23	8	0	0.246435	-1.020316	-0.898753
24	1	0	1.063816	-0.458699	-1.032830
25	8	0	2.654610	0.068340	-1.348251
26	6	0	3.587653	-0.224510	-0.541712
27	6	0	5.692953	-0.857369	1.226678
28	6	0	4.934407	0.257567	-0.778862
29	6	0	3.355902	-1.042985	0.632857
30	6	0	4.392750	-1.343970	1.486610
31	6	0	5.952748	-0.058215	0.091852
32	1	0	5.098576	0.869302	-1.660217
33	1	0	2.348358	-1.407222	0.806514
34	1	0	4.217162	-1.957911	2.364711
35	1	0	6.960032	0.304695	-0.088133
36	1	0	6.502471	-1.101270	1.907567

ACN-NQF-PhOH-T1-02-1-prod

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.686236	2.946619	-0.849276
2	6	0	-2.695898	2.695125	-0.483542
3	6	0	-0.166682	1.987618	0.466525
4	6	0	-2.420274	1.341652	-0.225622

5	6	0	-1.737642	3.676004	-0.275466
6	6	0	-0.467700	3.316174	0.204528
7	6	0	-1.124947	0.969688	0.257270
8	1	0	-1.968575	4.717658	-0.479859
9	1	0	0.286335	4.079479	0.374507
10	1	0	0.821479	1.743626	0.840727
11	6	0	-3.490921	0.350354	-0.457626
12	6	0	-3.106610	-1.003413	-0.145944
13	6	0	-1.850654	-1.369852	0.318688
14	6	0	-0.846002	-0.430903	0.516492
15	8	0	-3.956813	-2.040055	-0.296312
16	6	0	-3.283639	-3.254463	0.170377
17	1	0	-3.373202	-3.995495	-0.626246
18	1	0	-3.832305	-3.605334	1.048337
19	6	0	-1.819094	-2.868415	0.496364
20	1	0	-1.107574	-3.342677	-0.189480
21	1	0	-1.537440	-3.164672	1.512031
22	8	0	-4.631436	0.655418	-0.883830
23	8	0	0.333672	-0.901020	0.959890
24	1	0	1.074884	-0.243179	0.998986
25	8	0	2.661570	0.484872	1.140296
26	6	0	3.632429	0.062577	0.442204
27	6	0	5.815265	-0.850455	-1.092012
28	6	0	4.926029	0.712449	0.522726
29	6	0	3.493879	-1.071673	-0.450778
30	6	0	4.568189	-1.506317	-1.193123
31	6	0	5.983167	0.256991	-0.231650
32	1	0	5.019528	1.560502	1.193510
33	1	0	2.524213	-1.556180	-0.505790
34	1	0	4.463576	-2.355868	-1.860954
35	1	0	6.950882	0.745261	-0.170358
36	1	0	6.655110	-1.202288	-1.682957

ACN-NQF-PhOH-T1-02-2-prod

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.288829	-0.673065	-0.633517
2	6	0	4.383376	-1.186489	-0.325938
3	6	0	2.023599	-2.460009	0.466751
4	6	0	3.217585	-0.419369	-0.157466
5	6	0	4.374656	-2.556351	-0.105593
6	6	0	3.187048	-3.194807	0.292940
7	6	0	2.012812	-1.065722	0.246945
8	1	0	5.283948	-3.135468	-0.240553
9	1	0	3.178568	-4.267315	0.465997

10	1	0	1.106004	-2.949791	0.773611
11	6	0	3.271927	1.035336	-0.398700
12	6	0	2.013269	1.707292	-0.188521
13	6	0	0.830194	1.081018	0.203881
14	6	0	0.799696	-0.290855	0.421427
15	8	0	1.889734	3.038667	-0.368495
16	6	0	0.547926	3.431214	0.058862
17	1	0	0.144056	4.089570	-0.711839
18	1	0	0.659957	3.994163	0.990159
19	6	0	-0.261916	2.128634	0.255240
20	1	0	-0.994863	1.981791	-0.546914
21	1	0	-0.814093	2.134871	1.199071
22	8	0	4.314532	1.638446	-0.752812
23	8	0	-0.294971	-0.975164	0.793224
24	1	0	-1.100478	-0.402306	0.917212
25	8	0	-2.660661	0.263374	1.196951
26	6	0	-3.643488	-0.108364	0.486556
27	6	0	-5.852197	-0.908023	-1.073675
28	6	0	-4.965717	0.434213	0.730011
29	6	0	-3.490162	-1.075909	-0.582816
30	6	0	-4.577212	-1.456708	-1.336044
31	6	0	-6.035338	0.035640	-0.038909
32	1	0	-5.070013	1.156971	1.532893
33	1	0	-2.499594	-1.482679	-0.760269
34	1	0	-4.461175	-2.181135	-2.136304
35	1	0	-7.024632	0.443333	0.144707
36	1	0	-6.701941	-1.215984	-1.674892

Atomic coordinates of optimized NQP-Phenol structures [(u)b3lyp/6-31g(d) scrf=(iefpcm,solvent=acetonitrile)]

Ground state S_0 complexes

ACN-NQP-PhOH-S0-01-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.023435	1.962799	-0.648830
2	6	0	-0.027260	2.261664	-0.341666
3	6	0	2.542317	3.020491	0.464909
4	6	0	0.971375	1.292440	-0.188029
5	6	0	0.259473	3.603773	-0.091849
6	6	0	1.542752	3.983219	0.310124
7	6	0	2.264950	1.675554	0.219542
8	1	0	-0.518196	4.352115	-0.209858
9	1	0	1.764947	5.028375	0.503797

10	1	0	3.543898	3.297570	0.775697
11	6	0	0.672612	-0.134026	-0.445235
12	6	0	1.767114	-1.126494	-0.207510
13	6	0	3.028961	-0.758074	0.148406
14	6	0	3.347952	0.657259	0.385129
15	8	0	4.486203	0.997619	0.714153
16	8	0	1.361983	-2.390136	-0.408307
17	6	0	3.718609	-3.094179	-0.390134
18	1	0	3.795304	-3.000581	-1.479799
19	6	0	4.128421	-1.780104	0.285721
20	1	0	5.047546	-1.378920	-0.153729
21	1	0	4.350531	-1.945691	1.348915
22	8	0	-0.423448	-0.535940	-0.838566
23	1	0	-2.089529	0.114948	-1.208192
24	8	0	-2.970387	0.515592	-1.374595
25	6	0	-3.893395	-0.012790	-0.518498
26	6	0	-5.877259	-1.030222	1.184988
27	6	0	-5.200595	0.489149	-0.582279
28	6	0	-3.579576	-1.026085	0.398775
29	6	0	-4.572864	-1.526805	1.242851
30	6	0	-6.182356	-0.020507	0.266563
31	1	0	-5.428106	1.273634	-1.298338
32	1	0	-2.566672	-1.417192	0.443008
33	1	0	-4.320042	-2.312622	1.950223
34	1	0	-7.193069	0.375560	0.209137
35	1	0	-6.645235	-1.423958	1.844434
36	1	0	4.375374	-3.914822	-0.084211
37	6	0	2.284172	-3.439783	-0.019237
38	1	0	2.179384	-3.583915	1.062884
39	1	0	1.920084	-4.331256	-0.532036

ACN-NQP-PhOH-S0-01-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.321564	-3.020919	-0.110805
2	6	0	-1.374842	-2.764120	-0.074519
3	6	0	-4.080975	-2.056643	0.017177
4	6	0	-1.745492	-1.415300	-0.049136
5	6	0	-2.355224	-3.755937	-0.055296
6	6	0	-3.706794	-3.401975	-0.010326
7	6	0	-3.107020	-1.057790	-0.001827
8	1	0	-2.066423	-4.802307	-0.076252
9	1	0	-4.469936	-4.174388	0.003871
10	1	0	-5.125517	-1.766651	0.054979
11	6	0	-0.705097	-0.365373	-0.079397

12	6	0	-1.157630	1.058482	-0.071184
13	6	0	-2.469193	1.413545	0.010241
14	6	0	-3.516330	0.380215	0.040350
15	8	0	-4.706246	0.694988	0.103413
16	8	0	-0.128695	1.917308	-0.135796
17	6	0	-1.669977	3.727639	0.488824
18	1	0	-1.876175	4.788636	0.315489
19	1	0	-1.445930	3.606132	1.555081
20	6	0	-2.875127	2.862344	0.099180
21	1	0	-3.291553	3.191415	-0.862732
22	1	0	-3.685855	2.963342	0.827979
23	8	0	0.496722	-0.634556	-0.114835
24	1	0	1.941236	0.560440	-0.169672
25	8	0	2.769526	1.086661	-0.220484
26	6	0	3.862498	0.289479	-0.077105
27	6	0	6.202431	-1.241658	0.207256
28	6	0	5.122473	0.906016	-0.124662
29	6	0	3.778405	-1.098690	0.113269
30	6	0	4.946419	-1.851255	0.253574
31	6	0	6.279684	0.141967	0.016782
32	1	0	5.173867	1.981075	-0.272475
33	1	0	2.804339	-1.577362	0.148337
34	1	0	4.868439	-2.925802	0.400369
35	1	0	7.249109	0.632656	-0.022089
36	1	0	7.106478	-1.833611	0.317241
37	6	0	-0.451816	3.318750	-0.326259
38	1	0	-0.622014	3.472000	-1.398589
39	1	0	0.452694	3.851972	-0.030758

ACN-NQP-PhOH-S0-02-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.526881	3.330411	0.715638
2	6	0	-2.524166	3.041288	0.419259
3	6	0	0.046164	2.242742	-0.342854
4	6	0	-2.251772	1.689725	0.192884
5	6	0	-1.515198	3.992608	0.267053
6	6	0	-0.231724	3.591814	-0.111712
7	6	0	-0.959218	1.283328	-0.194730
8	1	0	-1.728677	5.042165	0.445174
9	1	0	0.556054	4.329999	-0.228159
10	1	0	1.043356	1.933978	-0.635474
11	6	0	-3.334440	0.690264	0.374683
12	6	0	-2.973245	-0.751384	0.158475
13	6	0	-1.735856	-1.146176	-0.257285

14	6	0	-0.674771	-0.158189	-0.452853
15	8	0	-3.998879	-1.574923	0.403102
16	6	0	-2.751002	-3.378970	-0.710273
17	1	0	-3.211625	-3.156235	-1.679942
18	6	0	-1.442027	-2.596319	-0.552622
19	1	0	-0.833748	-2.662695	-1.460220
20	1	0	-0.830919	-3.025157	0.253268
21	8	0	-4.475131	1.001129	0.692033
22	8	0	0.445055	-0.537841	-0.832811
23	1	0	2.085495	0.105371	-1.179609
24	8	0	2.973891	0.488822	-1.359029
25	6	0	3.893014	-0.030955	-0.495130
26	6	0	5.871404	-1.035588	1.223947
27	6	0	5.209629	0.442747	-0.583405
28	6	0	3.567675	-1.009744	0.455521
29	6	0	4.557978	-1.504237	1.306659
30	6	0	6.188296	-0.060163	0.272998
31	1	0	5.446730	1.200488	-1.324769
32	1	0	2.547582	-1.378553	0.518632
33	1	0	4.295753	-2.263164	2.039596
34	1	0	7.206025	0.314087	0.195815
35	1	0	6.636991	-1.424297	1.889162
36	1	0	-2.570253	-4.458004	-0.673094
37	6	0	-3.718763	-2.999622	0.399986
38	1	0	-4.695697	-3.471962	0.288023
39	1	0	-3.311566	-3.252957	1.385994

ACN-NQP-PhOH-S0-02-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.835329	-2.211435	-0.389821
2	6	0	3.781854	-2.362366	-0.179249
3	6	0	1.057054	-2.699045	0.359041
4	6	0	2.947220	-1.246167	-0.076392
5	6	0	3.256165	-3.644077	-0.014283
6	6	0	1.894848	-3.811188	0.254709
7	6	0	1.575809	-1.412609	0.194651
8	1	0	3.905701	-4.510273	-0.095783
9	1	0	1.484883	-4.808352	0.383839
10	1	0	-0.000074	-2.816618	0.570431
11	6	0	3.513680	0.112133	-0.260830
12	6	0	2.558813	1.268855	-0.155382
13	6	0	1.238620	1.115346	0.154645
14	6	0	0.679902	-0.226494	0.315429
15	8	0	3.160681	2.441279	-0.382709

16	6	0	2.307476	3.610350	-0.494881
17	1	0	2.981778	4.457346	-0.361528
18	6	0	0.344039	2.314469	0.355587
19	1	0	-0.342707	2.419809	-0.494664
20	1	0	-0.288146	2.150092	1.234598
21	8	0	4.699554	0.310390	-0.489785
22	8	0	-0.527651	-0.392972	0.554512
23	1	0	-2.004570	0.636057	0.469495
24	8	0	-2.821279	1.184336	0.431561
25	6	0	-3.898226	0.411565	0.120596
26	6	0	-6.192165	-1.080469	-0.512188
27	6	0	-5.148298	1.041951	0.031660
28	6	0	-3.799356	-0.969336	-0.108644
29	6	0	-4.944877	-1.703419	-0.422621
30	6	0	-6.283545	0.296284	-0.282708
31	1	0	-5.210386	2.111461	0.211699
32	1	0	-2.830150	-1.455228	-0.037838
33	1	0	-4.856838	-2.772840	-0.597874
34	1	0	-7.246811	0.796023	-0.348419
35	1	0	-7.079245	-1.657603	-0.756687
36	1	0	1.911333	3.627366	-1.517107
37	6	0	1.186919	3.583611	0.532166
38	1	0	0.571686	4.481329	0.415279
39	1	0	1.622192	3.612237	1.537927

Relaxed T_1 complexes

ACN-NQP-PhOH-T1-01-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.102847	1.806891	-0.779761
2	6	0	-0.134259	2.158621	-0.443586
3	6	0	2.362829	3.063716	0.432397
4	6	0	0.900607	1.221569	-0.235955
5	6	0	0.078261	3.508886	-0.219671
6	6	0	1.334359	3.967277	0.220631
7	6	0	2.168330	1.687753	0.210964
8	1	0	-0.728779	4.216903	-0.384500
9	1	0	1.495590	5.027165	0.394195
10	1	0	3.338495	3.393640	0.772744
11	6	0	0.643557	-0.202141	-0.480234
12	6	0	1.743471	-1.101333	-0.226964
13	6	0	3.066877	-0.639206	0.214546
14	6	0	3.292281	0.767805	0.448995
15	8	0	4.418608	1.159790	0.844568

16	8	0	1.501607	-2.382033	-0.439015
17	6	0	3.913343	-2.905891	-0.387862
18	1	0	4.054727	-2.714880	-1.457653
19	6	0	4.158723	-1.628956	0.423433
20	1	0	5.119983	-1.158665	0.197410
21	1	0	4.195738	-1.877071	1.498811
22	8	0	-0.462725	-0.667061	-0.880090
23	1	0	-2.051237	-0.065094	-1.248036
24	8	0	-2.955972	0.266375	-1.474430
25	6	0	-3.857236	-0.146147	-0.540153
26	6	0	-5.803461	-0.941268	1.322624
27	6	0	-5.191202	0.258553	-0.696223
28	6	0	-3.499739	-0.951584	0.552363
29	6	0	-4.473634	-1.342585	1.473133
30	6	0	-6.153147	-0.139406	0.231257
31	1	0	-5.454413	0.881343	-1.546564
32	1	0	-2.466594	-1.267331	0.666865
33	1	0	-4.185775	-1.967229	2.315259
34	1	0	-7.183820	0.180490	0.099413
35	1	0	-6.556046	-1.248910	2.042910
36	1	0	4.618386	-3.690416	-0.096957
37	6	0	2.504046	-3.404009	-0.136466
38	1	0	2.347517	-3.681055	0.911775
39	1	0	2.222893	-4.242297	-0.773558

ACN-NQP-PhOH-T1-01-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.514938	-2.997248	-0.811743
2	6	0	-1.509923	-2.702464	-0.496847
3	6	0	-4.064252	-1.898059	0.313210
4	6	0	-1.765909	-1.331533	-0.287022
5	6	0	-2.507351	-3.643970	-0.305680
6	6	0	-3.793677	-3.240668	0.102328
7	6	0	-3.064577	-0.925974	0.123756
8	1	0	-2.297383	-4.696850	-0.470456
9	1	0	-4.572604	-3.982676	0.251436
10	1	0	-5.048174	-1.566417	0.627440
11	6	0	-0.683420	-0.367445	-0.503901
12	6	0	-1.014628	1.019030	-0.294469
13	6	0	-2.340784	1.461249	0.160174
14	6	0	-3.390672	0.489523	0.362956
15	8	0	-4.529236	0.871351	0.731031
16	8	0	-0.043623	1.884275	-0.520349
17	6	0	-1.277247	3.660075	0.665631

18	1	0	-1.444064	4.741414	0.665653
19	1	0	-0.873291	3.387827	1.647283
20	6	0	-2.587192	2.910059	0.397473
21	1	0	-3.073796	3.327187	-0.501679
22	1	0	-3.315828	3.024886	1.205190
23	8	0	0.475747	-0.721268	-0.870069
24	1	0	1.913709	0.292567	-0.919354
25	8	0	2.776471	0.774865	-0.988653
26	6	0	3.757602	0.098359	-0.338622
27	6	0	5.873334	-1.209361	0.974836
28	6	0	5.044172	0.661163	-0.330647
29	6	0	3.535947	-1.124970	0.315657
30	6	0	4.592227	-1.766988	0.964726
31	6	0	6.089090	0.008808	0.321835
32	1	0	5.204134	1.607400	-0.840079
33	1	0	2.541209	-1.561072	0.306097
34	1	0	4.407505	-2.713579	1.467095
35	1	0	7.079888	0.456663	0.319524
36	1	0	6.690147	-1.714323	1.482548
37	6	0	-0.268276	3.326044	-0.415086
38	1	0	-0.602987	3.652836	-1.405600
39	1	0	0.724806	3.730333	-0.220879

ACN-NQP-PhOH-T1-02-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.394896	3.382398	0.693450
2	6	0	-2.407026	3.055637	0.387538
3	6	0	0.123687	2.161485	-0.400359
4	6	0	-2.200886	1.677794	0.182376
5	6	0	-1.376404	3.961993	0.203108
6	6	0	-0.101930	3.511448	-0.193138
7	6	0	-0.913540	1.221590	-0.218344
8	1	0	-1.549892	5.022119	0.364053
9	1	0	0.704955	4.224086	-0.336163
10	1	0	1.103717	1.811381	-0.704078
11	6	0	-3.335954	0.764297	0.402366
12	6	0	-3.055138	-0.638911	0.203302
13	6	0	-1.746078	-1.128311	-0.250675
14	6	0	-0.654985	-0.201716	-0.446554
15	8	0	-4.056228	-1.471919	0.436527
16	6	0	-2.889802	-3.294655	-0.739198
17	1	0	-3.306178	-3.019313	-1.714797
18	6	0	-1.553366	-2.582267	-0.505962
19	1	0	-0.850808	-2.716473	-1.333491

20	1	0	-1.051508	-3.015129	0.377694
21	8	0	-4.472098	1.157664	0.759066
22	8	0	0.463865	-0.665412	-0.813396
23	1	0	2.076530	-0.055790	-1.195404
24	8	0	2.972102	0.285761	-1.431353
25	6	0	3.892959	-0.133344	-0.517982
26	6	0	5.877533	-0.939389	1.297498
27	6	0	5.221781	0.277527	-0.697168
28	6	0	3.559179	-0.949796	0.573278
29	6	0	4.552359	-1.346476	1.470868
30	6	0	6.203136	-0.125964	0.207252
31	1	0	5.465793	0.909067	-1.546714
32	1	0	2.529586	-1.270006	0.706988
33	1	0	4.283210	-1.979827	2.312588
34	1	0	7.229945	0.198523	0.058067
35	1	0	6.645205	-1.251417	1.999700
36	1	0	-2.754189	-4.380267	-0.732751
37	6	0	-3.864337	-2.918219	0.358804
38	1	0	-4.868619	-3.308805	0.195847
39	1	0	-3.511113	-3.235637	1.346195

ACN-NQP-PhOH-T1-02-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.600045	-1.977559	-1.011099
2	6	0	3.664946	-2.179435	-0.499936
3	6	0	1.241435	-2.650756	0.817253
4	6	0	2.814787	-1.092200	-0.219903
5	6	0	3.313571	-3.466591	-0.127905
6	6	0	2.093373	-3.704631	0.536126
7	6	0	1.581029	-1.333089	0.444668
8	1	0	3.980513	-4.295677	-0.346351
9	1	0	1.822689	-4.715421	0.826827
10	1	0	0.298829	-2.814763	1.328099
11	6	0	3.233835	0.254905	-0.642743
12	6	0	2.303879	1.319670	-0.339841
13	6	0	1.066495	1.103058	0.419982
14	6	0	0.657565	-0.241045	0.756033
15	8	0	2.633790	2.523055	-0.782136
16	6	0	1.712828	3.645145	-0.622753
17	1	0	2.344677	4.524542	-0.744653
18	6	0	0.253569	2.271389	0.860210
19	1	0	-0.666417	2.292064	0.249992
20	1	0	-0.096498	2.104035	1.884936
21	8	0	4.304608	0.479324	-1.255319

22	8	0	-0.450485	-0.444011	1.334161
23	1	0	-1.954876	0.453597	1.133516
24	8	0	-2.775903	0.979181	0.970883
25	6	0	-3.685052	0.240219	0.277226
26	6	0	-5.640588	-1.190500	-1.141354
27	6	0	-4.900034	0.853575	-0.063274
28	6	0	-3.450433	-1.092086	-0.096286
29	6	0	-4.428518	-1.796402	-0.800573
30	6	0	-5.867388	0.138143	-0.767300
31	1	0	-5.067660	1.885458	0.231982
32	1	0	-2.507404	-1.562563	0.167973
33	1	0	-4.237045	-2.828176	-1.084746
34	1	0	-6.805388	0.623308	-1.025332
35	1	0	-6.396870	-1.743871	-1.690500
36	1	0	1.004734	3.592489	-1.457261
37	6	0	1.016751	3.592106	0.722406
38	1	0	0.332638	4.442053	0.801723
39	1	0	1.759641	3.691252	1.521972

Optimized T1-TS for H-abstraction

ACN-NQP-PhOH-T1-TS-01-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.203490	2.662945	1.353628
2	6	0	0.699219	2.611216	0.755153
3	6	0	3.054648	2.474429	-0.744591
4	6	0	1.236468	1.343190	0.432234
5	6	0	1.319966	3.773554	0.329440
6	6	0	2.504134	3.708087	-0.430156
7	6	0	2.442336	1.282128	-0.321428
8	1	0	0.894153	4.739406	0.587113
9	1	0	2.987693	4.622443	-0.762464
10	1	0	3.970456	2.398559	-1.321689
11	6	0	0.573772	0.128134	0.879625
12	6	0	1.212369	-1.121558	0.566494
13	6	0	2.400373	-1.208949	-0.199646
14	6	0	3.059025	-0.010741	-0.664537
15	8	0	4.119833	-0.081036	-1.338901
16	8	0	0.566656	-2.210928	1.026210
17	6	0	1.923667	-3.653326	-0.428094
18	1	0	1.192615	-3.589128	-1.243117
19	1	0	2.385822	-4.644684	-0.477566
20	6	0	2.975090	-2.547602	-0.563248
21	1	0	3.387956	-2.496568	-1.575798

22	1	0	3.831745	-2.767730	0.093720
23	8	0	-0.528047	0.130890	1.547230
24	1	0	-1.666514	0.912052	1.135977
25	8	0	-2.529476	1.423036	0.812040
26	6	0	-3.387455	0.637265	0.193681
27	6	0	-5.296600	-0.942986	-1.106269
28	6	0	-4.564689	1.233528	-0.343741
29	6	0	-3.178553	-0.767471	0.059160
30	6	0	-4.131763	-1.535613	-0.583806
31	6	0	-5.503271	0.444568	-0.979778
32	1	0	-4.697105	2.304330	-0.230014
33	1	0	-2.269534	-1.200268	0.463771
34	1	0	-3.978587	-2.605152	-0.689938
35	1	0	-6.403835	0.894900	-1.385389
36	1	0	-6.035383	-1.555938	-1.612559
37	6	0	1.206447	-3.504363	0.902706
38	1	0	0.395822	-4.223716	1.030058
39	1	0	1.905355	-3.608103	1.742448

ACN-NQP-PhOH-T1-TS-01-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.537016	-2.960241	-1.099186
2	6	0	-1.491295	-2.668524	-0.673835
3	6	0	-3.939984	-1.876965	0.421285
4	6	0	-1.698645	-1.307148	-0.359707
5	6	0	-2.485667	-3.605322	-0.446759
6	6	0	-3.719962	-3.208922	0.105035
7	6	0	-2.944387	-0.908618	0.197223
8	1	0	-2.313911	-4.649125	-0.695219
9	1	0	-4.497529	-3.946945	0.281505
10	1	0	-4.882688	-1.549288	0.847441
11	6	0	-0.639992	-0.337119	-0.599834
12	6	0	-0.924520	1.031399	-0.271299
13	6	0	-2.160762	1.457917	0.279180
14	6	0	-3.209104	0.499432	0.540766
15	8	0	-4.304079	0.867658	1.042042
16	8	0	0.068571	1.891752	-0.566197
17	6	0	-1.425642	3.802322	-0.205416
18	1	0	-1.703052	3.836694	-1.265754
19	1	0	-1.445347	4.829291	0.173621
20	6	0	-2.398547	2.910148	0.573810
21	1	0	-3.442932	3.154082	0.354912
22	1	0	-2.275738	3.084754	1.654932
23	8	0	0.499133	-0.693672	-1.076383

24	1	0	1.697959	0.204558	-1.009156
25	8	0	2.604913	0.717550	-0.970363
26	6	0	3.543352	0.059962	-0.314698
27	6	0	5.619406	-1.248518	1.034846
28	6	0	4.822143	0.673356	-0.200564
29	6	0	3.319812	-1.219901	0.267899
30	6	0	4.355853	-1.856867	0.928690
31	6	0	5.841865	0.018839	0.465685
32	1	0	4.966844	1.650014	-0.650728
33	1	0	2.336955	-1.669900	0.177840
34	1	0	4.189478	-2.833670	1.372735
35	1	0	6.818819	0.484806	0.550022
36	1	0	6.422712	-1.755572	1.559835
37	6	0	-0.015575	3.252166	-0.073766
38	1	0	0.713515	3.802930	-0.669601
39	1	0	0.313548	3.245496	0.972766

ACN-NQP-PhOH-T1-TS-02-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.987055	3.052173	0.184958
2	6	0	2.916998	2.872229	0.185744
3	6	0	0.173132	2.345406	0.193567
4	6	0	2.474283	1.537687	0.091512
5	6	0	2.013316	3.916748	0.282255
6	6	0	0.629795	3.649115	0.289980
7	6	0	1.076458	1.264917	0.083854
8	1	0	2.368484	4.941024	0.355001
9	1	0	-0.080913	4.466682	0.372693
10	1	0	-0.892185	2.146075	0.207155
11	6	0	3.473930	0.465048	0.009168
12	6	0	2.943394	-0.882475	-0.078684
13	6	0	1.551918	-1.170019	-0.057789
14	6	0	0.596472	-0.110371	-0.008650
15	8	0	3.878435	-1.844745	-0.167092
16	6	0	2.193329	-3.562401	0.313377
17	1	0	2.383726	-3.504260	1.391840
18	1	0	1.917519	-4.596640	0.083163
19	6	0	1.074643	-2.595228	-0.085898
20	1	0	0.199916	-2.696521	0.564330
21	1	0	0.716952	-2.837446	-1.099231
22	8	0	4.711568	0.686765	0.005898
23	8	0	-0.656478	-0.415471	-0.030274
24	1	0	-1.800364	0.342767	-0.497976
25	8	0	-2.678553	0.779498	-0.869425

26	6	0	-3.775080	0.217768	-0.394900
27	6	0	-6.162844	-0.899946	0.541672
28	6	0	-5.024294	0.664338	-0.910831
29	6	0	-3.742209	-0.797766	0.603787
30	6	0	-4.929804	-1.344888	1.054280
31	6	0	-6.198711	0.107408	-0.440887
32	1	0	-5.020501	1.438191	-1.671281
33	1	0	-2.781648	-1.122755	0.988769
34	1	0	-4.911012	-2.119841	1.814366
35	1	0	-7.152891	0.445939	-0.832387
36	1	0	-7.088477	-1.332818	0.907307
37	6	0	3.461970	-3.204146	-0.439937
38	1	0	3.318314	-3.294513	-1.524272
39	1	0	4.316081	-3.816977	-0.147003

ACN-NQP-PhOH-T1-TS-02-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.663354	-1.960544	-0.838973
2	6	0	3.691813	-2.171535	-0.404155
3	6	0	1.174828	-2.659606	0.713334
4	6	0	2.820076	-1.087816	-0.177071
5	6	0	3.316668	-3.464319	-0.078175
6	6	0	2.047955	-3.709819	0.485962
7	6	0	1.538844	-1.334806	0.388001
8	1	0	3.999708	-4.290639	-0.255265
9	1	0	1.756010	-4.724511	0.742353
10	1	0	0.196536	-2.832785	1.148757
11	6	0	3.252777	0.267220	-0.540751
12	6	0	2.291294	1.323358	-0.280821
13	6	0	1.032106	1.095606	0.342922
14	6	0	0.610100	-0.237450	0.636535
15	8	0	2.695778	2.550071	-0.653424
16	6	0	0.908135	3.586555	0.653824
17	1	0	0.208798	4.428585	0.662979
18	1	0	1.572661	3.701030	1.518471
19	6	0	0.158307	2.252911	0.728853
20	1	0	-0.726533	2.277365	0.068609
21	1	0	-0.245400	2.084091	1.734018
22	8	0	4.372060	0.509770	-1.059265
23	8	0	-0.552110	-0.481554	1.137716
24	1	0	-1.745493	0.355125	0.990918
25	8	0	-2.638703	0.894942	0.887642
26	6	0	-3.584117	0.219775	0.257797
27	6	0	-5.669674	-1.128943	-1.030098

28	6	0	-4.842175	0.858180	0.074788
29	6	0	-3.383033	-1.103109	-0.227888
30	6	0	-4.424543	-1.760812	-0.858158
31	6	0	-5.868019	0.182377	-0.559516
32	1	0	-4.967539	1.868244	0.450670
33	1	0	-2.411652	-1.566947	-0.093170
34	1	0	-4.276891	-2.770261	-1.229494
35	1	0	-6.830783	0.665047	-0.695604
36	1	0	-6.477185	-1.651828	-1.532523
37	6	0	1.734269	3.630963	-0.618859
38	1	0	2.335438	4.537495	-0.702720
39	1	0	1.099093	3.542328	-1.509515

Relaxed Triplet Radical Pair Products

ACN-NQP-PhOH-T1-01-1-prod

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.055485	1.966424	0.796007
2	6	0	-0.066958	2.239807	0.444489
3	6	0	2.463747	3.021201	-0.451859
4	6	0	0.930197	1.251358	0.250267
5	6	0	0.203921	3.575726	0.192534
6	6	0	1.472930	3.975038	-0.259934
7	6	0	2.217565	1.663607	-0.203597
8	1	0	-0.574571	4.317171	0.349062
9	1	0	1.677275	5.023782	-0.455580
10	1	0	3.453957	3.300241	-0.796961
11	6	0	0.704352	-0.144885	0.502923
12	6	0	1.761764	-1.087944	0.321367
13	6	0	3.012714	-0.710628	-0.138736
14	6	0	3.300400	0.680360	-0.417177
15	8	0	4.428195	1.039038	-0.831223
16	8	0	1.423752	-2.374336	0.613322
17	6	0	3.498074	-3.148980	-0.439061
18	1	0	2.978843	-3.310547	-1.391736
19	1	0	4.282621	-3.909198	-0.359484
20	6	0	4.090177	-1.736631	-0.385284
21	1	0	4.614393	-1.488585	-1.314428
22	1	0	4.849520	-1.676883	0.408190
23	8	0	-0.454216	-0.659719	0.937430
24	1	0	-1.223848	-0.031995	0.948134
25	8	0	-2.838669	0.614652	1.020295
26	6	0	-3.782835	0.065442	0.376015
27	6	0	-5.909072	-1.130389	-1.037899

28	6	0	-5.109675	0.649996	0.387276
29	6	0	-3.580599	-1.152892	-0.384355
30	6	0	-4.628253	-1.725368	-1.069041
31	6	0	-6.138734	0.056497	-0.307465
32	1	0	-5.250050	1.561827	0.958895
33	1	0	-2.586238	-1.588003	-0.388446
34	1	0	-4.476441	-2.637851	-1.637396
35	1	0	-7.131506	0.495743	-0.298402
36	1	0	-6.727233	-1.591485	-1.582322
37	6	0	2.505884	-3.323542	0.700804
38	1	0	2.020409	-4.301644	0.686229
39	1	0	3.002260	-3.192715	1.672034

ACN-NQP-PhOH-T1-01-2-prod

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.086147	-3.123416	-0.868896
2	6	0	-1.995908	-2.648436	-0.518090
3	6	0	-4.335955	-1.405336	0.389175
4	6	0	-1.996468	-1.254621	-0.277302
5	6	0	-3.144752	-3.394516	-0.307303
6	6	0	-4.322095	-2.773769	0.148434
7	6	0	-3.187060	-0.627784	0.183577
8	1	0	-3.134378	-4.464523	-0.495348
9	1	0	-5.218915	-3.364725	0.311518
10	1	0	-5.233014	-0.905814	0.740669
11	6	0	-0.824030	-0.456405	-0.477697
12	6	0	-0.857847	0.941709	-0.223882
13	6	0	-2.007347	1.584290	0.206129
14	6	0	-3.222600	0.828650	0.439921
15	8	0	-4.269002	1.392485	0.837685
16	8	0	0.326428	1.574727	-0.458204
17	6	0	-0.805504	3.735730	-0.251418
18	1	0	-0.951429	3.787109	-1.337291
19	1	0	-0.665663	4.760364	0.109480
20	6	0	-2.017351	3.076992	0.419779
21	1	0	-2.956200	3.488772	0.034086
22	1	0	-2.017277	3.298281	1.497171
23	8	0	0.290025	-1.067363	-0.900621
24	1	0	1.067781	-0.452553	-1.004746
25	8	0	2.740318	0.004729	-1.343176
26	6	0	3.662193	-0.311275	-0.533918
27	6	0	5.741376	-0.998186	1.247437
28	6	0	5.025719	0.122601	-0.770794
29	6	0	3.401061	-1.110964	0.647839

30	6	0	4.425022	-1.438453	1.507774
31	6	0	6.030663	-0.218951	0.106029
32	1	0	5.213322	0.720329	-1.657171
33	1	0	2.381296	-1.439892	0.820633
34	1	0	4.226622	-2.038069	2.391005
35	1	0	7.050080	0.108406	-0.074294
36	1	0	6.540522	-1.262594	1.932973
37	6	0	0.448589	2.923745	0.039764
38	1	0	1.333068	3.326122	-0.457670
39	1	0	0.641945	2.875455	1.119700

ACN-NQP-PhOH-T1-02-1-prod

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.374388	3.330873	-0.862750
2	6	0	-2.398077	3.032462	-0.495134
3	6	0	0.092328	2.202443	0.465848
4	6	0	-2.186293	1.667987	-0.230657
5	6	0	-1.393074	3.963998	-0.287167
6	6	0	-0.142970	3.541989	0.199420
7	6	0	-0.917568	1.233328	0.252675
8	1	0	-1.570311	5.015576	-0.494327
9	1	0	0.646401	4.268401	0.370987
10	1	0	1.065718	1.912345	0.845077
11	6	0	-3.290576	0.722101	-0.443121
12	6	0	-3.012238	-0.670929	-0.118597
13	6	0	-1.758696	-1.109999	0.314850
14	6	0	-0.724853	-0.175174	0.502159
15	8	0	-4.068129	-1.497167	-0.298485
16	6	0	-2.593625	-3.440562	-0.091771
17	1	0	-2.456838	-3.478803	-1.179419
18	1	0	-2.554811	-4.469651	0.280823
19	6	0	-1.500118	-2.583696	0.554875
20	1	0	-0.515142	-2.851086	0.159293
21	1	0	-1.455953	-2.783186	1.634678
22	8	0	-4.413249	1.083851	-0.867534
23	8	0	0.439523	-0.689875	0.941820
24	1	0	1.212561	-0.069968	0.945485
25	8	0	2.849961	0.561089	1.052832
26	6	0	3.801071	0.032656	0.402179
27	6	0	5.942079	-1.120295	-1.025759
28	6	0	5.132635	0.603614	0.461981
29	6	0	3.602391	-1.149170	-0.414497
30	6	0	4.656913	-1.701203	-1.105428
31	6	0	6.168835	0.031194	-0.239977

32	1	0	5.270925	1.488215	1.075392
33	1	0	2.604311	-1.573780	-0.454513
34	1	0	4.507349	-2.586483	-1.715867
35	1	0	7.165100	0.460175	-0.194173
36	1	0	6.765827	-1.564844	-1.575502
37	6	0	-3.956133	-2.840931	0.214392
38	1	0	-4.135604	-2.809544	1.297450
39	1	0	-4.772200	-3.390300	-0.259324

ACN-NQP-PhOH-T1-02-2-prod

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.918295	-1.728033	-0.730236
2	6	0	3.941523	-2.010176	-0.350725
3	6	0	1.403764	-2.682032	0.619488
4	6	0	2.988254	-0.993843	-0.160302
5	6	0	3.636661	-3.331613	-0.061390
6	6	0	2.359262	-3.666903	0.425917
7	6	0	1.699919	-1.329711	0.334031
8	1	0	4.381255	-4.108411	-0.211643
9	1	0	2.119675	-4.702469	0.651008
10	1	0	0.419051	-2.937899	0.994113
11	6	0	3.331104	0.396296	-0.485179
12	6	0	2.284491	1.386208	-0.254407
13	6	0	1.023629	1.063696	0.269865
14	6	0	0.728139	-0.283105	0.534183
15	8	0	2.656653	2.647043	-0.569514
16	6	0	0.714876	3.528972	0.626842
17	1	0	-0.023774	4.337090	0.616925
18	1	0	1.302692	3.629824	1.547151
19	6	0	0.023898	2.162095	0.579815
20	1	0	-0.774766	2.176419	-0.173703
21	1	0	-0.468206	1.959798	1.537546
22	8	0	4.452966	0.725233	-0.937375
23	8	0	-0.459306	-0.688608	1.023762
24	1	0	-1.188401	-0.016293	0.969966
25	8	0	-2.778312	0.717369	0.918274
26	6	0	-3.733200	0.138867	0.317482
27	6	0	-5.883848	-1.116911	-1.007931
28	6	0	-5.047254	0.751031	0.277130
29	6	0	-3.557886	-1.139532	-0.345027
30	6	0	-4.616713	-1.740409	-0.987309
31	6	0	-6.088222	0.127875	-0.372902
32	1	0	-5.168767	1.707571	0.775395
33	1	0	-2.573838	-1.596055	-0.311302

34	1	0	-4.483927	-2.697626	-1.482223
35	1	0	-7.070967	0.588453	-0.401486
36	1	0	-6.710901	-1.600707	-1.518195
37	6	0	1.638546	3.668660	-0.570487
38	1	0	2.188353	4.611912	-0.568271
39	1	0	1.076581	3.591345	-1.510781

Atomic coordinates of optimized NQF-Indole structures [(u)b3lyp/6-31+g(d) scrf=(iefpcm,solvent=acetonitrile)]

Ground state S_0 complex

ACN-NQF-indole-S0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.807011	-2.457755	0.192778
2	6	0	2.658053	-1.071085	0.078171
3	6	0	3.793955	-0.229717	0.160522
4	6	0	5.053364	-0.798211	0.356458
5	6	0	5.194615	-2.185836	0.470599
6	6	0	4.072999	-3.015404	0.388710
7	1	0	1.927354	-3.090003	0.127039
8	1	0	5.919104	-0.146742	0.418610
9	1	0	6.180203	-2.616240	0.622986
10	1	0	4.181833	-4.092337	0.476756
11	6	0	3.668344	1.264494	0.040680
12	6	0	2.326774	1.786758	-0.156759
13	6	0	1.245500	0.975184	-0.235557
14	6	0	1.300908	-0.501856	-0.131109
15	8	0	4.657358	2.003375	0.107572
16	8	0	0.284360	-1.191577	-0.214941
17	6	0	-3.533566	0.012109	1.478566
18	6	0	-4.719566	0.333227	2.134940
19	6	0	-5.969637	0.234566	1.479779
20	6	0	-6.055938	-0.187352	0.155935
21	6	0	-4.873784	-0.519254	-0.536664
22	6	0	-3.623082	-0.411934	0.144445
23	1	0	-2.573388	0.087120	1.982639
24	1	0	-4.683928	0.665308	3.169506
25	1	0	-6.875570	0.493042	2.022612
26	1	0	-7.022305	-0.260263	-0.338164
27	7	0	-2.635334	-0.791423	-0.739908
28	1	0	-1.635642	-0.813039	-0.544590
29	6	0	-4.580614	-0.978865	-1.867354

30	1	0	-5.289114	-1.172882	-2.662287
31	6	0	-3.214332	-1.129364	-1.945068
32	1	0	-2.597101	-1.454621	-2.772033
33	6	0	1.877289	3.216782	-0.318282
34	1	0	2.146094	3.832696	0.546718
35	1	0	2.322567	3.684042	-1.203922
36	6	0	0.341460	3.046518	-0.457105
37	1	0	-0.219598	3.482644	0.371025
38	1	0	-0.056509	3.411123	-1.404889
39	8	0	0.071386	1.592213	-0.421976

Relaxed T_1 complex

ACN-NQF-indole-T1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.928584	-2.341735	0.360761
2	6	0	2.592078	-0.988677	0.131644
3	6	0	3.631024	-0.006577	0.142219
4	6	0	4.955779	-0.419367	0.380168
5	6	0	5.266562	-1.756231	0.603475
6	6	0	4.243218	-2.723607	0.593737
7	1	0	2.132386	-3.079903	0.351296
8	1	0	5.734362	0.337906	0.385443
9	1	0	6.296362	-2.053486	0.785429
10	1	0	4.481646	-3.769966	0.768590
11	6	0	3.338531	1.430529	-0.083876
12	6	0	1.967781	1.741068	-0.329604
13	6	0	0.982364	0.774892	-0.335936
14	6	0	1.198210	-0.618061	-0.113924
15	8	0	4.251242	2.311597	-0.052672
16	8	0	0.247387	-1.487113	-0.125731
17	6	0	-3.102199	0.457659	1.228158
18	6	0	-4.261876	1.063920	1.779236
19	6	0	-5.545186	0.773598	1.301496
20	6	0	-5.728864	-0.134876	0.252532
21	6	0	-4.589769	-0.752382	-0.309703
22	6	0	-3.295031	-0.436351	0.199584
23	1	0	-2.112983	0.699750	1.600579
24	1	0	-4.141936	1.772855	2.592706
25	1	0	-6.405951	1.259318	1.749589
26	1	0	-6.722439	-0.362172	-0.121715
27	7	0	-2.352882	-1.187148	-0.530121
28	1	0	-1.293216	-1.190895	-0.373771
29	6	0	-4.400058	-1.692932	-1.346087

30	1	0	-5.150539	-2.163739	-1.966813
31	6	0	-2.989091	-1.922375	-1.431436
32	1	0	-2.454626	-2.581735	-2.102450
33	6	0	1.320405	3.088280	-0.543457
34	1	0	1.347535	3.696378	0.371320
35	1	0	1.798271	3.675307	-1.335299
36	6	0	-0.121454	2.682288	-0.925607
37	1	0	-0.898493	3.235742	-0.395512
38	1	0	-0.296236	2.755043	-2.004273
39	8	0	-0.272382	1.271173	-0.560915

Optimized T1-TS for H-abstraction

ACN-NQF-indole-T1-TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.712930	-2.410195	0.010053
2	6	0	2.476716	-1.016844	-0.017974
3	6	0	3.577407	-0.124782	0.164612
4	6	0	4.862206	-0.657689	0.366005
5	6	0	5.075745	-2.032428	0.390801
6	6	0	3.992341	-2.911856	0.211447
7	1	0	1.873417	-3.083749	-0.128436
8	1	0	5.688420	0.033679	0.502493
9	1	0	6.076799	-2.425443	0.548160
10	1	0	4.154992	-3.986481	0.230088
11	6	0	3.385455	1.347502	0.141186
12	6	0	2.039487	1.786369	-0.050752
13	6	0	0.992013	0.904833	-0.225789
14	6	0	1.130692	-0.508288	-0.226240
15	8	0	4.353509	2.148599	0.279185
16	8	0	0.135120	-1.342308	-0.396526
17	6	0	-3.170071	-0.462975	1.492550
18	6	0	-4.364250	-0.208592	2.214215
19	6	0	-5.592156	-0.038048	1.565442
20	6	0	-5.680403	-0.114705	0.168167
21	6	0	-4.504983	-0.366738	-0.564491
22	6	0	-3.262919	-0.536944	0.118940
23	1	0	-2.225595	-0.593254	2.011649
24	1	0	-4.318246	-0.146177	3.297410
25	1	0	-6.485634	0.154807	2.151048
26	1	0	-6.633173	0.016428	-0.336583
27	7	0	-2.244031	-0.779905	-0.828667
28	1	0	-0.994587	-0.967335	-0.589236
29	6	0	-4.214374	-0.510664	-1.944155

30	1	0	-4.898676	-0.449695	-2.780594
31	6	0	-2.801975	-0.762843	-2.026510
32	1	0	-2.216373	-0.924808	-2.923407
33	6	0	1.507403	3.193072	-0.167144
34	1	0	1.811437	3.835683	0.665999
35	1	0	1.852785	3.675288	-1.091661
36	6	0	-0.018670	2.948645	-0.175290
37	1	0	-0.477935	3.175491	0.792110
38	1	0	-0.553160	3.479390	-0.964646
39	8	0	-0.213856	1.514277	-0.414429

Relaxed Triplet Radical Pair Products

ACN-NQF-indole-T1-prod

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.777974	-2.419704	-0.002476
2	6	0	2.547586	-1.024760	-0.010165
3	6	0	3.652636	-0.137007	0.164841
4	6	0	4.937356	-0.673351	0.341311
5	6	0	5.147066	-2.049900	0.347254
6	6	0	4.060090	-2.924409	0.174311
7	1	0	1.937882	-3.092987	-0.136240
8	1	0	5.767253	0.013912	0.474250
9	1	0	6.149135	-2.446835	0.485378
10	1	0	4.220506	-3.999231	0.178400
11	6	0	3.459782	1.336975	0.167137
12	6	0	2.114300	1.783679	-0.029826
13	6	0	1.062766	0.904832	-0.194913
14	6	0	1.215095	-0.499012	-0.196360
15	8	0	4.421999	2.132922	0.336107
16	8	0	0.211669	-1.360988	-0.354613
17	6	0	-3.313039	-0.435966	1.492001
18	6	0	-4.509028	-0.190694	2.212090
19	6	0	-5.736225	-0.034048	1.559295
20	6	0	-5.819189	-0.116503	0.160035
21	6	0	-4.641733	-0.359314	-0.566108
22	6	0	-3.396030	-0.515560	0.116322
23	1	0	-2.367407	-0.556453	2.012544
24	1	0	-4.466953	-0.124334	3.295523
25	1	0	-6.633937	0.152519	2.141080
26	1	0	-6.773096	0.004201	-0.346086
27	7	0	-2.355083	-0.752407	-0.813459
28	1	0	-0.719397	-0.965948	-0.504904

29	6	0	-4.337486	-0.506759	-1.947049
30	1	0	-5.017253	-0.455646	-2.788657
31	6	0	-2.919232	-0.744236	-2.008525
32	1	0	-2.334606	-0.903220	-2.908006
33	6	0	1.567823	3.188437	-0.032343
34	1	0	1.644198	3.646517	0.962672
35	1	0	2.091186	3.847165	-0.733378
36	6	0	0.097919	2.953927	-0.452516
37	1	0	-0.633576	3.448461	0.187941
38	1	0	-0.084616	3.228253	-1.495742
39	8	0	-0.146709	1.509405	-0.343551

Atomic coordinates of optimized structures NQF-Indole π-π structures [(u)b3lyp/6-31+g(d) scrf=(iefpcm,solvent=acetonitrile)]

ACN-NQF-indole-T1-Pi-complex01

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.775150	-1.235552	-0.490834
2	6	0	2.651521	-0.598638	0.077091
3	6	0	2.555424	0.824572	0.002260
4	6	0	3.583897	1.548780	-0.632957
5	6	0	4.680709	0.901169	-1.185611
6	6	0	4.775765	-0.502012	-1.113241
7	1	0	3.838580	-2.317440	-0.428068
8	1	0	3.496857	2.629964	-0.679892
9	1	0	5.463985	1.475780	-1.672771
10	1	0	5.633322	-1.011542	-1.544915
11	6	0	1.409167	1.561719	0.580828
12	6	0	0.403358	0.745248	1.189057
13	6	0	0.526351	-0.674650	1.263137
14	6	0	1.621861	-1.430487	0.733596
15	8	0	1.317511	2.821055	0.552072
16	8	0	1.697487	-2.689928	0.831207
17	6	0	-4.149243	-1.083895	-0.519641
18	6	0	-4.965006	0.027198	-0.269544
19	6	0	-4.496186	1.341518	-0.461967
20	6	0	-3.195996	1.583366	-0.906844
21	6	0	-2.352144	0.484512	-1.162286
22	6	0	-2.853323	-0.834279	-0.964216
23	1	0	-4.515713	-2.095523	-0.372061
24	1	0	-5.981786	-0.131239	0.078347
25	1	0	-5.159282	2.177934	-0.260381

26	1	0	-2.840373	2.598945	-1.058178
27	7	0	-1.825834	-1.715060	-1.287571
28	1	0	-1.880091	-2.724430	-1.235662
29	6	0	-0.994116	0.352838	-1.595639
30	1	0	-0.313734	1.144639	-1.875227
31	6	0	-0.722658	-1.014596	-1.663733
32	1	0	0.179024	-1.524798	-1.970528
33	6	0	-0.812001	1.157007	1.951401
34	1	0	-0.556351	1.833502	2.776996
35	1	0	-1.533598	1.692750	1.319285
36	6	0	-1.375776	-0.187706	2.452908
37	1	0	-1.371583	-0.284338	3.540525
38	1	0	-2.370954	-0.419696	2.070058
39	8	0	-0.478498	-1.235595	1.944581

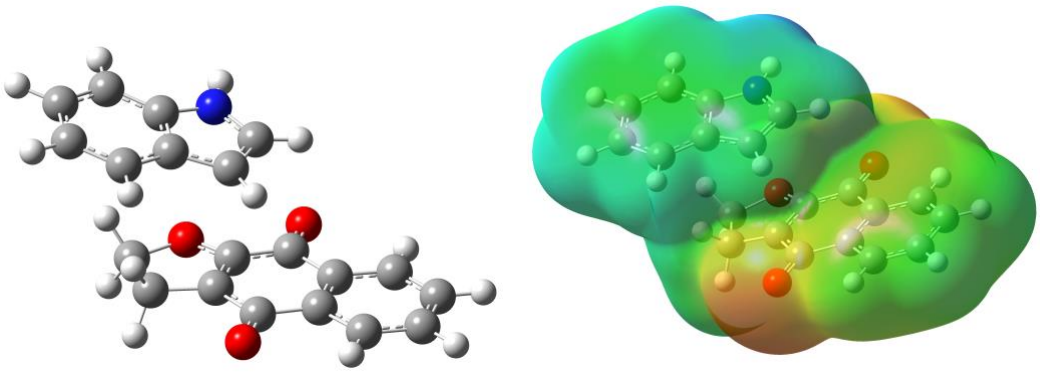
ACN-NQF-indole-T1-Pi-complex02

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.834182	-2.273401	-1.428370
2	6	0	-0.202656	-1.533193	-0.822051
3	6	0	-0.434797	-1.693089	0.578690
4	6	0	0.374227	-2.585471	1.310517
5	6	0	1.389143	-3.303434	0.693207
6	6	0	1.619659	-3.145182	-0.687573
7	1	0	1.002299	-2.144839	-2.492997
8	1	0	0.182646	-2.698317	2.373179
9	1	0	2.004076	-3.986584	1.273116
10	1	0	2.413014	-3.707154	-1.173626
11	6	0	-1.514339	-0.963366	1.280295
12	6	0	-2.279415	-0.075281	0.460812
13	6	0	-2.037145	0.060461	-0.939838
14	6	0	-1.014474	-0.630923	-1.663703
15	8	0	-1.760202	-1.118286	2.509967
16	8	0	-0.836281	-0.485768	-2.908267
17	6	0	3.244754	0.900569	1.122597
18	6	0	4.020235	0.874954	-0.043137
19	6	0	3.513441	1.334053	-1.276372
20	6	0	2.216211	1.830903	-1.378647
21	6	0	1.411712	1.868086	-0.221198
22	6	0	1.949351	1.397938	1.011932
23	1	0	3.641628	0.548472	2.070350
24	1	0	5.036169	0.493350	0.006674
25	1	0	4.147054	1.297984	-2.157968
26	1	0	1.828806	2.184523	-2.330108
27	7	0	0.960402	1.558885	1.978107

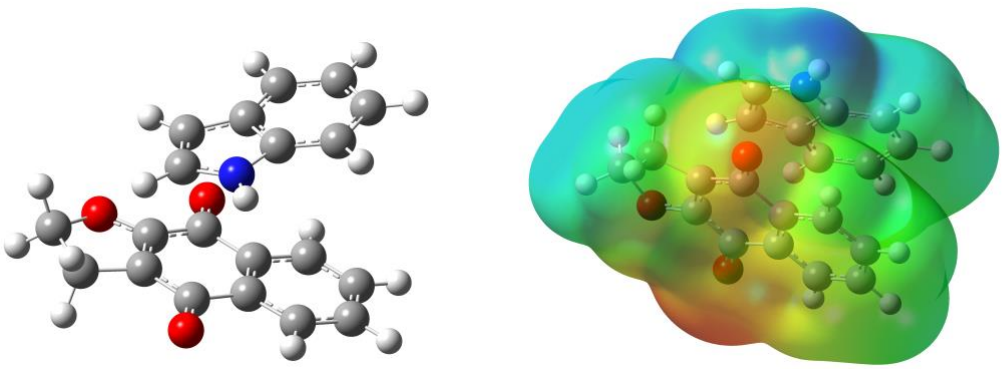
28	1	0	1.045017	1.301839	2.953107
29	6	0	0.078190	2.305543	0.046992
30	1	0	-0.614360	2.760508	-0.647175
31	6	0	-0.150935	2.097087	1.409534
32	1	0	-1.019927	2.329026	2.008098
33	6	0	-3.526767	0.681382	0.793826
34	1	0	-4.335567	-0.014398	1.058815
35	1	0	-3.408604	1.359901	1.645444
36	6	0	-3.827149	1.430641	-0.518753
37	1	0	-4.841726	1.291990	-0.894039
38	1	0	-3.602082	2.498753	-0.462296
39	8	0	-2.926245	0.866943	-1.532935

Optimized S_0 structures of NQF-Indole π–π complexes and Electrostatic Potential maps (Blue positive → green neutral → red negative charge)

ACN-NQF-indole-T1-Pi-complex01-631+Gd



ACN-NQF-indole-T1-Pi-complex02-631+Gd



Thermodynamics from calculations

NQF-Phenol calculations

B3LYP/6-31G(d)/IEFPCM=ACN	Energetic units = hartrees				Relative to ACN-NQF-PhOH-S0-01-1				Relative to ACN-NQF-PhOH-S0-02-2			
imaginary vibration (cm-1)			-1445.56		Energetic units = kcal				Energetic units = kcal			
Total Electronic Energy=	-995.2460093	-995.1878	-995.17993	-995.1981	0.00	36.53	41.47	30.06	1.42	37.95	42.89	31.49
Zero-point correction=	0.2795	0.277486	0.27225	0.27704	0.00	-1.26	-4.55	-1.54	0.00	-1.27	-4.55	-1.55
Thermal correction to Energy=	0.298141	0.29602	0.290419	0.295683	0.00	-1.33	-4.85	-1.54	0.04	-1.29	-4.80	-1.50
Thermal correction to Enthalpy=	0.299085	0.296965	0.291363	0.296627	0.00	-1.33	-4.85	-1.54	0.04	-1.29	-4.81	-1.50
Thermal correction to Gibbs Free Energy=	0.228325	0.225794	0.22058	0.225071	0.00	-1.59	-4.86	-2.04	-0.10	-1.69	-4.96	-2.14
Sum of electronic and zero-point Energies=	-994.966509	-994.91032	-994.90768	-994.92106	0.00	35.26	36.92	28.52	1.42	36.68	38.34	29.94
Sum of electronic and thermal Energies=	-994.947868	-994.89178	-994.88951	-994.90242	0.00	35.19	36.62	28.52	1.46	36.66	38.08	29.98
Sum of electronic and thermal Enthalpies=	-994.946924	-994.89084	-994.88856	-994.90147	0.00	35.19	36.62	28.52	1.46	36.66	38.08	29.98
Sum of electronic and thermal Free Energies=	-995.017684	-994.96201	-994.95935	-994.97303	0.00	34.94	36.61	28.02	1.32	36.26	37.93	29.34

ACN-NQF-PhOH-S0-01-1

ACN-NQF-PhOH-T1-01-1

ACN-NQF-PhOH-T1-TS-01-1

ACN-NQF-PhOH-T1-01-1-prod

					Relative to ACN-NQF-PhOH-S0-01-2				Relative to ACN-NQF-PhOH-S0-02-2			
imaginary vibration (cm-1)			-1017.67									
Total Electronic Energy=	-995.2465214	-995.18845	-995.18333	-995.20081	0.00	36.44	39.65	28.68	1.10	37.54	40.76	29.79
Zero-point correction=	0.279212	0.277266	0.272817	0.276956	0.00	-1.22	-4.01	-1.42	-0.18	-1.40	-4.20	-1.60
Thermal correction to Energy=	0.297939	0.295821	0.290831	0.295603	0.00	-1.33	-4.46	-1.47	-0.09	-1.42	-4.55	-1.55
Thermal correction to Enthalpy=	0.298883	0.296765	0.291776	0.296548	0.00	-1.33	-4.46	-1.47	-0.09	-1.42	-4.55	-1.55
Thermal correction to Gibbs Free Energy=	0.227542	0.225607	0.222458	0.224595	0.00	-1.21	-3.19	-1.85	-0.59	-1.81	-3.78	-2.44
Sum of electronic and zero-point Energies=	-994.967309	-994.91119	-994.91051	-994.92385	0.00	35.22	35.64	27.27	0.92	36.14	36.56	28.19
Sum of electronic and thermal Energies=	-994.948583	-994.89263	-994.8925	-994.90521	0.00	35.11	35.19	27.22	1.02	36.12	36.21	28.23
Sum of electronic and thermal Enthalpies=	-994.947638	-994.89169	-994.89155	-994.90426	0.00	35.11	35.19	27.22	1.02	36.12	36.21	28.23
Sum of electronic and thermal Free Energies=	-995.01898	-994.96285	-994.96087	-994.97621	0.00	35.22	36.46	26.84	0.51	35.73	36.97	27.35

ACN-NQF-PhOH-S0-01-2

ACN-NQF-PhOH-T1-01-2

ACN-NQF-PhOH-T1-TS-01-2

ACN-NQF-PhOH-T1-01-2-prod

					Relative to ACN-NQF-PhOH-S0-02-1				Relative to ACN-NQF-PhOH-S0-02-2			
imaginary vibration (cm-1)			-1331.6									
Total Electronic Energy=	-995.2475813	-995.1866	-995.18	-995.20158	0.00	38.27	42.40	28.87	0.44	38.70	42.84	29.30
Zero-point correction=	0.279562	0.277503	0.27251	0.277304	0.00	-1.29	-4.43	-1.42	0.04	-1.26	-4.39	-1.38
Thermal correction to Energy=	0.29817	0.296039	0.290642	0.295929	0.00	-1.34	-4.72	-1.41	0.06	-1.28	-4.66	-1.35
Thermal correction to Enthalpy=	0.299114	0.296983	0.291587	0.296873	0.00	-1.34	-4.72	-1.41	0.06	-1.28	-4.66	-1.35
Thermal correction to Gibbs Free Energy=	0.228232	0.225853	0.221213	0.22518	0.00	-1.49	-4.40	-1.92	-0.16	-1.65	-4.56	-2.07
Sum of electronic and zero-point Energies=	-994.968019	-994.9091	-994.90749	-994.92428	0.00	36.97	37.98	27.45	0.47	37.45	38.45	27.92
Sum of electronic and thermal Energies=	-994.949412	-994.89056	-994.88936	-994.90565	0.00	36.93	37.68	27.46	0.50	37.42	38.18	27.96
Sum of electronic and thermal Enthalpies=	-994.948467	-994.88962	-994.88842	-994.90471	0.00	36.93	37.68	27.46	0.50	37.42	38.18	27.96
Sum of electronic and thermal Free Energies=	-995.019349	-994.96075	-994.95879	-994.9764	0.00	36.77	38.00	26.95	0.28	37.05	38.28	27.23

ACN-NQF-PhOH-S0-02-1

ACN-NQF-PhOH-T1-02-1

ACN-NQF-PhOH-T1-TS-02-1

ACN-NQF-PhOH-T1-02-1-prod

					Relative to ACN-NQF-PhOH-S0-02-2				Relative to ACN-NQF-PhOH-S0-02-2			
imaginary vibration (cm-1)			-1084.22									
Total Electronic Energy=	-995.2482776	-995.18733	-995.18308	-995.204	0.00	38.25	40.91	27.79	0.00	38.25	40.91	27.79
Zero-point correction=	0.279505	0.27731	0.272759	0.277559	0.00	-1.38	-4.23	-1.22	0.00	-1.38	-4.23	-1.22
Thermal correction to Energy=	0.298076	0.29582	0.290706	0.296078	0.00	-1.42	-4.62	-1.25	0.00	-1.42	-4.62	-1.25
Thermal correction to Enthalpy=	0.299021	0.296764	0.29165	0.297022	0.00	-1.42	-4.63	-1.25	0.00	-1.42	-4.63	-1.25
Thermal correction to Gibbs Free Energy=	0.228484	0.225734	0.22272	0.225689	0.00	-1.73	-3.62	-1.75	0.00	-1.73	-3.62	-1.75
Sum of electronic and zero-point Energies=	-994.968773	-994.91002	-994.91032	-994.92644	0.00	36.87	36.68	26.57	0.00	36.87	36.68	26.57
Sum of electronic and thermal Energies=	-994.950201	-994.89151	-994.89237	-994.90792	0.00	36.83	36.29	26.53	0.00	36.83	36.29	26.53
Sum of electronic and thermal Enthalpies=	-994.949257	-994.89056	-994.89143	-994.90698	0.00	36.83	36.29	26.53	0.00	36.83	36.29	26.53
Sum of electronic and thermal Free Energies=	-995.019794	-994.96159	-994.96036	-994.97831	0.00	36.52	37.29	26.03	0.00	36.52	37.29	26.03

ACN-NQF-PhOH-S0-02-2

ACN-NQF-PhOH-T1-02-2

ACN-NQF-PhOH-T1-TS-02-2

ACN-NQF-PhOH-T1-02-2-prod

NQF-Phenol calculations

B3LYP/6-311++G(d,p)//6-31G(d)/IEFPCM=ACN

					Relative to ACN-NQF-PhOH-S0-01-1-6311				Relative to ACN-NQF-PhOH-S0-01-2-6311			
imaginary vibration (cm-1)												
Total Electronic Energy=	-995.520914	-995.4633	-995.45561	-995.47311	0.00	36.16	40.98	30.00	0.53	36.68	41.50	30.52
Zero-point correction=	0.2795	0.277486	0.27225	0.27704	0.00	-1.26	-4.55	-1.54	0.18	-1.08	-4.37	-1.36
Thermal correction to Energy=	0.298141	0.29602	0.290419	0.295683	0.00	-1.33	-4.85	-1.54	0.13	-1.20	-4.72	-1.42
Thermal correction to Enthalpy=	0.299085	0.296965	0.291363	0.296627	0.00	-1.33	-4.85	-1.54	0.13	-1.20	-4.72	-1.42
Thermal correction to Gibbs Free Energy=	0.228325	0.225794	0.22058	0.225071	0.00	-1.59	-4.86	-2.04	0.49	-1.10	-4.37	-1.55
Sum of electronic and zero-point Energies=	-995.241414	-995.18581	-995.18336	-995.19607	0.00	34.89	36.43	28.45	0.71	35.60	37.13	29.16
Sum of electronic and thermal Energies=	-995.222773	-995.16728	-995.16519	-995.17743	0.00	34.82	36.13	28.45	0.65	35.48	36.78	29.11
Sum of electronic and thermal Enthalpies=	-995.221829	-995.16633	-995.16425	-995.17649	0.00	34.82	36.13	28.45	1.24	36.07	37.38	29.70
Sum of electronic and thermal Free Energies=	-995.292589	-995.2375	-995.23503	-995.24804	0.00	34.57	36.12	27.95	1.02	35.58	37.13	28.97
	ACN-NQF-PhOH-S0-01-1-6311											
		ACN-NQF-PhOH-T1-01-1-6311										
			ACN-NQF-PhOH-T1-TS-01-1-6311									
				ACN-NQF-PhOH-T1-01-1-prod-6311								

					Relative to ACN-NQF-PhOH-S0-01-2-6311				Relative to ACN-NQF-PhOH-S0-01-2-6311			
imaginary vibration (cm-1)												
Total Electronic Energy=	-995.521752	-995.46412	-995.45861	-995.47541	0.00	36.16	39.62	29.08	0.00	36.16	39.62	29.08
Zero-point correction=	0.279212	0.277266	0.272817	0.276956	0.00	-1.22	-4.01	-1.42	0.00	-1.22	-4.01	-1.42
Thermal correction to Energy=	0.297939	0.295821	0.290831	0.295603	0.00	-1.33	-4.46	-1.47	0.00	-1.33	-4.46	-1.47
Thermal correction to Enthalpy=	0.298883	0.296765	0.291776	0.296548	0.00	-1.33	-4.46	-1.47	0.00	-1.33	-4.46	-1.47
Thermal correction to Gibbs Free Energy=	0.227542	0.225607	0.222458	0.224595	0.00	-1.21	-3.19	-1.85	0.00	-1.21	-3.19	-1.85
Sum of electronic and zero-point Energies=	-995.24254	-995.18685	-995.1858	-995.19845	0.00	34.94	35.61	27.66	0.00	34.94	35.61	27.66
Sum of electronic and thermal Energies=	-995.223813	-995.1683	-995.16778	-995.17981	0.00	34.83	35.16	27.61	0.00	34.83	35.16	27.61
Sum of electronic and thermal Enthalpies=	-995.223813	-995.1683	-995.16778	-995.17981	0.00	34.83	35.16	27.61	0.00	34.83	35.16	27.61
Sum of electronic and thermal Free Energies=	-995.29421	-995.23851	-995.23615	-995.25081	0.00	34.95	36.43	27.23	0.00	34.95	36.43	27.23
	ACN-NQF-PhOH-S0-01-2-6311											
		ACN-NQF-PhOH-T1-01-2-6311										
			ACN-NQF-PhOH-T1-TS-01-2-6311									
				ACN-NQF-PhOH-T1-01-2-prod-6311								

					Relative to ACN-NQF-PhOH-S0-02-1-6311				Relative to ACN-NQF-PhOH-S0-01-2-6311			
imaginary vibration (cm-1)												
Total Electronic Energy=	-995.5220994	-995.46239	-995.45632	-995.47633	0.00	37.47	41.28	28.72	-0.22	37.25	41.06	28.50
Zero-point correction=	0.279562	0.277503	0.27251	0.277304	0.00	-1.29	-4.43	-1.42	0.22	-1.07	-4.21	-1.20
Thermal correction to Energy=	0.29817	0.296039	0.290642	0.295929	0.00	-1.34	-4.72	-1.41	0.14	-1.19	-4.58	-1.26
Thermal correction to Enthalpy=	0.299114	0.296983	0.291587	0.296873	0.00	-1.34	-4.72	-1.41	0.14	-1.19	-4.58	-1.26
Thermal correction to Gibbs Free Energy=	0.228232	0.225853	0.221213	0.22518	0.00	-1.49	-4.40	-1.92	0.43	-1.06	-3.97	-1.48
Sum of electronic and zero-point Energies=	-995.2425374	-995.18489	-995.18381	-995.19902	0.00	36.17	36.85	27.31	0.00	36.17	36.85	27.31
Sum of electronic and thermal Energies=	-995.2239294	-995.16635	-995.16568	-995.1804	0.00	36.13	36.55	27.32	-0.07	36.06	36.48	27.24
Sum of electronic and thermal Enthalpies=	-995.2229854	-995.16541	-995.16473	-995.17945	0.00	36.13	36.55	27.32	0.52	36.65	37.07	27.84
Sum of electronic and thermal Free Energies=	-995.2938674	-995.23654	-995.23511	-995.25115	0.00	35.97	36.87	26.81	0.21	36.19	37.09	27.02
	ACN-NQF-PhOH-S0-02-1-6311	ACN-NQF-PhOH-T1-02-1-6311	ACN-NQF-PhOH-T1-TS-02-1-6311	ACN-NQF-PhOH-T1-02-1-prod-6311								

					Relative to ACN-NQF-PhOH-S0-02-2-6311				Relative to ACN-NQF-PhOH-S0-01-2-6311			
imaginary vibration (cm-1)												
Total Electronic Energy=	-995.5226646	-995.46266	-995.45857	-995.47833	0.00	37.66	40.22	27.82	-0.57	37.08	39.65	27.25
Zero-point correction=	0.279505	0.27731	0.272759	0.277559	0.00	-1.38	-4.23	-1.22	0.18	-1.19	-4.05	-1.04
Thermal correction to Energy=	0.298076	0.29582	0.290706	0.296078	0.00	-1.42	-4.62	-1.25	0.09	-1.33	-4.54	-1.17
Thermal correction to Enthalpy=	0.299021	0.296764	0.29165	0.297022	0.00	-1.42	-4.63	-1.25	0.09	-1.33	-4.54	-1.17
Thermal correction to Gibbs Free Energy=	0.228484	0.225734	0.22272	0.225689	0.00	-1.73	-3.62	-1.75	0.59	-1.13	-3.03	-1.16
Sum of electronic and zero-point Energies=	-995.2431596	-995.18535	-995.18581	-995.20077	0.00	36.28	35.99	26.60	-0.39	35.89	35.60	26.21
Sum of electronic and thermal Energies=	-995.2245886	-995.16684	-995.16787	-995.18225	0.00	36.24	35.59	26.57	-0.49	35.75	35.11	26.08
Sum of electronic and thermal Enthalpies=	-995.2236436	-995.16589	-995.16692	-995.1813	0.00	36.24	35.59	26.57	0.11	36.35	35.70	26.67
Sum of electronic and thermal Free Energies=	-995.2941806	-995.23692	-995.23585	-995.25264	0.00	35.93	36.60	26.07	0.02	35.95	36.62	26.09
	ACN-NQF-PhOH-S0-02-2-6311	ACN-NQF-PhOH-T1-02-2-6311	ACN-NQF-PhOH-T1-TS-02-2-6311	ACN-NQF-PhOH-T1-02-2-prod-6311								

NQP-Phenol calculations

B3LYP/6-31G(d)/IEFPCM=ACN

	Energies in hartrees				Relative to ACN-NQP-PhOH-S0-01-1 Energies in kcal				Relative to ACN-NQP-PhOH-S0-01-2 Energies in kcal			
imaginary vibration (cm-1)			-1305.55									
Total Electronic Energy=	-1034.5695	-1034.5043	-1034.4985	-1034.5186	0.00	40.92	44.59	31.95	0.73	41.65	45.33	32.68
Zero-point correction=	0.309115	0.306978	0.302281	0.306705	0.00	-1.34	-4.29	-1.51	0.16	-1.18	-4.13	-1.35
Thermal correction to Energy=	0.328527	0.326427	0.321208	0.326115	0.00	-1.32	-4.59	-1.51	0.10	-1.22	-4.49	-1.41
Thermal correction to Enthalpy=	0.329471	0.327371	0.322153	0.327059	0.00	-1.32	-4.59	-1.51	0.10	-1.22	-4.49	-1.41
Thermal correction to Gibbs Free Energy=	0.25718	0.254497	0.250868	0.254341	0.00	-1.68	-3.96	-1.78	0.87	-0.82	-3.09	-0.92
Sum of electronic and zero-point Energies=	-1034.2604	-1034.1973	-1034.1958	-1034.2119	0.00	39.58	40.56	30.43	0.89	40.47	41.45	31.33
Sum of electronic and thermal Energies=	-1034.241	-1034.1779	-1034.1768	-1034.1925	0.00	39.60	40.26	30.43	0.84	40.43	41.09	31.27
Sum of electronic and thermal Enthalpies=	-1034.24	-1034.1769	-1034.1759	-1034.1915	0.00	39.60	40.26	30.43	0.84	40.43	41.09	31.27
Sum of electronic and thermal Free Energies=	-1034.3123	-1034.2498	-1034.2472	-1034.2643	0.00	39.23	40.89	30.17	1.60	40.83	42.49	31.76

ACN-NQP-PhOH-S0-01-1

ACN-NQP-PhOH-T1-01-1

ACN-NQP-PhOH-T1-TS-01-1

ACN-NQP-PhOH-T1-01-1-prod

					Relative to ACN-NQP-PhOH-S0-01-2				Relative to ACN-NQP-PhOH-S0-01-2			
imaginary vibration (cm-1)			-793.09									
Total Electronic Energy=	-1034.5707	-1034.5053	-1034.5019	-1034.5227	0.00	41.00	43.19	30.14	0.00	41.00	43.19	30.14
Zero-point correction=	0.308863	0.30671	0.302887	0.30653	0.00	-1.35	-3.75	-1.46	0.00	-1.35	-3.75	-1.46
Thermal correction to Energy=	0.328364	0.326212	0.321747	0.325998	0.00	-1.35	-4.15	-1.48	0.00	-1.35	-4.15	-1.48
Thermal correction to Enthalpy=	0.329308	0.327156	0.322691	0.326942	0.00	-1.35	-4.15	-1.48	0.00	-1.35	-4.15	-1.48
Thermal correction to Gibbs Free Energy=	0.2558	0.253982	0.251895	0.253883	0.00	-1.14	-2.45	-1.20	0.00	-1.14	-2.45	-1.20
Sum of electronic and zero-point Energies=	-1034.2618	-1034.1986	-1034.199	-1034.2161	0.00	39.65	39.44	28.68	0.00	39.65	39.44	28.68
Sum of electronic and thermal Energies=	-1034.2423	-1034.1791	-1034.1801	-1034.1967	0.00	39.65	39.04	28.66	0.00	39.65	39.04	28.66
Sum of electronic and thermal Enthalpies=	-1034.2414	-1034.1782	-1034.1792	-1034.1957	0.00	39.65	39.04	28.66	0.00	39.65	39.04	28.66
Sum of electronic and thermal Free Energies=	-1034.3149	-1034.2514	-1034.25	-1034.2688	0.00	39.86	40.74	28.94	0.00	39.86	40.74	28.94

ACN-NQP-PhOH-S0-01-2

ACN-NQP-PhOH-T1-01-2

ACN-NQP-PhOH-T1-TS-01-2

ACN-NQP-PhOH-T1-01-2-prod

imaginary vibration (cm-1)			-1344.6		Relative to ACN-NQP-PhOH-S0-02-1				Relative to ACN-NQP-PhOH-S0-01-2			
Total Electronic Energy=	-1034.5707	-1034.5029	-1034.4969	-1034.5205	0.00	42.56	46.31	31.48	-0.02	42.55	46.29	31.46
Zero-point correction=	0.309158	0.306812	0.302084	0.30685	0.00	-1.47	-4.44	-1.45	0.19	-1.29	-4.25	-1.26
Thermal correction to Energy=	0.328544	0.326377	0.321131	0.326263	0.00	-1.36	-4.65	-1.43	0.11	-1.25	-4.54	-1.32
Thermal correction to Enthalpy=	0.329488	0.327321	0.322075	0.327207	0.00	-1.36	-4.65	-1.43	0.11	-1.25	-4.54	-1.32
Thermal correction to Gibbs Free Energy=	0.257254	0.253527	0.250282	0.25425	0.00	-2.34	-4.37	-1.89	0.91	-1.43	-3.46	-0.97
Sum of electronic and zero-point Energies=	-1034.2616	-1034.1961	-1034.1948	-1034.2137	0.00	41.09	41.87	30.03	0.17	41.26	42.04	30.20
Sum of electronic and thermal Energies=	-1034.2422	-1034.1765	-1034.1758	-1034.1943	0.00	41.20	41.65	30.05	0.10	41.30	41.75	30.15
Sum of electronic and thermal Enthalpies=	-1034.2412	-1034.1756	-1034.1748	-1034.1933	0.00	41.20	41.65	30.05	0.10	41.30	41.75	30.15
Sum of electronic and thermal Free Energies=	-1034.3135	-1034.2494	-1034.2466	-1034.2663	0.00	40.23	41.93	29.60	0.89	41.12	42.83	30.49

ACN-NQP-PhOH-S0-02-1

ACN-NQP-PhOH-T1-02-1

ACN-NQP-PhOH-T1-TS-02-1

ACN-NQP-PhOH-T1-02-1-prod

imaginary vibration (cm-1)			-901.95		Relative to ACN-NQP-PhOH-S0-02-2				Relative to ACN-NQP-PhOH-S0-01-2			
Total Electronic Energy=	-1034.5705	-1034.5025	-1034.499	-1034.5212	0.00	42.65	44.85	30.92	0.11	42.76	44.96	31.02
Zero-point correction=	0.309111	0.306688	0.302622	0.306905	0.00	-1.52	-4.07	-1.38	0.16	-1.36	-3.92	-1.23
Thermal correction to Energy=	0.328477	0.32618	0.321442	0.326273	0.00	-1.44	-4.41	-1.38	0.07	-1.37	-4.34	-1.31
Thermal correction to Enthalpy=	0.329422	0.327124	0.322386	0.327217	0.00	-1.44	-4.42	-1.38	0.07	-1.37	-4.34	-1.31
Thermal correction to Gibbs Free Energy=	0.257604	0.253624	0.25156	0.254748	0.00	-2.50	-3.79	-1.79	1.13	-1.37	-2.66	-0.66
Sum of electronic and zero-point Energies=	-1034.2614	-1034.1959	-1034.1964	-1034.2143	0.00	41.13	40.78	29.53	0.26	41.39	41.04	29.80
Sum of electronic and thermal Energies=	-1034.242	-1034.1764	-1034.1776	-1034.195	0.00	41.21	40.44	29.53	0.18	41.39	40.62	29.71
Sum of electronic and thermal Enthalpies=	-1034.2411	-1034.1754	-1034.1767	-1034.194	0.00	41.21	40.44	29.53	0.18	41.39	40.62	29.71
Sum of electronic and thermal Free Energies=	-1034.3129	-1034.2489	-1034.2475	-1034.2665	0.00	40.15	41.06	29.12	1.24	41.39	42.30	30.36

ACN-NQP-PhOH-S0-02-2

ACN-NQP-PhOH-T1-02-2

ACN-NQP-PhOH-T1-TS-02-2

ACN-NQP-PhOH-T1-02-2-prod

NQP-Phenol calculations
B3LYP/6-311++G(d,p)//6-31G(d)/IEFPCM=ACN

					Relative to ACN-NQP-PhOH-S0-01-1-6311				Relative to ACN-NQP-PhOH-S0-01-2-6311			
Total Electronic Energy=	-1034.8537	-1034.7891	-1034.7826	-1034.8027	0.00	40.54	44.64	32.02	0.94	41.48	45.58	32.96
Zero-point correction=	0.309115	0.306978	0.302281	0.306705	0.00	-1.34	-4.29	-1.51	0.16	-1.18	-4.13	-1.35
Thermal correction to Energy=	0.328527	0.326427	0.321208	0.326115	0.00	-1.32	-4.59	-1.51	0.10	-1.22	-4.49	-1.41
Thermal correction to Enthalpy=	0.329471	0.327371	0.322153	0.327059	0.00	-1.32	-4.59	-1.51	0.10	-1.22	-4.49	-1.41
Thermal correction to Gibbs Free Energy=	0.25718	0.254497	0.250868	0.254341	0.00	-1.68	-3.96	-1.78	0.87	-0.82	-3.09	-0.92
Sum of electronic and zero-point Energies=	-1034.5446	-1034.4821	-1034.4803	-1034.496	0.00	39.20	40.35	30.51	1.10	40.29	41.45	31.61
Sum of electronic and thermal Energies=	-1034.5252	-1034.4627	-1034.4614	-1034.4766	0.00	39.22	40.05	30.51	1.04	40.26	41.09	31.55
Sum of electronic and thermal Enthalpies=	-1034.5242	-1034.4617	-1034.4604	-1034.4756	0.00	39.22	40.05	30.51	1.04	40.26	41.09	31.55
Sum of electronic and thermal Free Energies=	-1034.5965	-1034.5346	-1034.5317	-1034.5483	0.00	38.85	40.68	30.24	1.80	40.66	42.48	32.05

ACN-NQP-PhOH-S0-01-1-6311

ACN-NQP-PhOH-T1-01-1-6311

ACN-NQP-PhOH-T1-TS-01-1-6311

ACN-NQP-PhOH-T1-01-1-prod-6311

					Relative to ACN-NQP-PhOH-S0-01-2-6311				Relative to ACN-NQP-PhOH-S0-01-2-6311			
Total Electronic Energy=	-1034.8552	-1034.7902	-1034.786	-1034.8064	0.00	40.78	43.44	30.66	0.00	40.78	43.44	30.66
Zero-point correction=	0.308863	0.30671	0.302887	0.30653	0.00	-1.35	-3.75	-1.46	0.00	-1.35	-3.75	-1.46
Thermal correction to Energy=	0.328364	0.326212	0.321747	0.325998	0.00	-1.35	-4.15	-1.48	0.00	-1.35	-4.15	-1.48
Thermal correction to Enthalpy=	0.329308	0.327156	0.322691	0.326942	0.00	-1.35	-4.15	-1.48	0.00	-1.35	-4.15	-1.48
Thermal correction to Gibbs Free Energy=	0.2558	0.253982	0.251895	0.253883	0.00	-1.14	-2.45	-1.20	0.00	-1.14	-2.45	-1.20
Sum of electronic and zero-point Energies=	-1034.5464	-1034.4835	-1034.4831	-1034.4998	0.00	39.43	39.69	29.19	0.00	39.43	39.69	29.19
Sum of electronic and thermal Energies=	-1034.5269	-1034.464	-1034.4642	-1034.4804	0.00	39.43	39.29	29.17	0.00	39.43	39.29	29.17
Sum of electronic and thermal Enthalpies=	-1034.5259	-1034.4631	-1034.4633	-1034.4794	0.00	39.43	39.29	29.17	0.00	39.43	39.29	29.17
Sum of electronic and thermal Free Energies=	-1034.5994	-1034.5362	-1034.5341	-1034.5525	0.00	39.64	40.99	29.46	0.00	39.64	40.99	29.46

ACN-NQP-PhOH-S0-01-2-6311

ACN-NQP-PhOH-T1-01-2-6311

ACN-NQP-PhOH-T1-TS-01-2-6311

ACN-NQP-PhOH-T1-01-2-prod-6311

					Relative to ACN-NQP-PhOH-S0-02-1-6311				Relative to ACN-NQP-PhOH-S0-01-2-6311			
Total Electronic Energy=	-1034.8547	-1034.7882	-1034.7829	-1034.8049	0.00	41.77	45.06	31.25	0.31	42.08	45.37	31.56
Zero-point correction=	0.309158	0.306812	0.302084	0.30685	0.00	-1.47	-4.44	-1.45	0.19	-1.29	-4.25	-1.26
Thermal correction to Energy=	0.328544	0.326377	0.321131	0.326263	0.00	-1.36	-4.65	-1.43	0.11	-1.25	-4.54	-1.32
Thermal correction to Enthalpy=	0.329488	0.327321	0.322075	0.327207	0.00	-1.36	-4.65	-1.43	0.11	-1.25	-4.54	-1.32
Thermal correction to Gibbs Free Energy=	0.257254	0.253527	0.250282	0.25425	0.00	-2.34	-4.37	-1.89	0.91	-1.43	-3.46	-0.97
Sum of electronic and zero-point Energies=	-1034.5456	-1034.4813	-1034.4808	-1034.4981	0.00	40.30	40.62	29.80	0.50	40.80	41.12	30.30
Sum of electronic and thermal Energies=	-1034.5262	-1034.4618	-1034.4618	-1034.4787	0.00	40.41	40.41	29.82	0.43	40.84	40.83	30.25
Sum of electronic and thermal Enthalpies=	-1034.5252	-1034.4608	-1034.4608	-1034.4777	0.00	40.41	40.41	29.82	0.43	40.84	40.83	30.25
Sum of electronic and thermal Free Energies=	-1034.5975	-1034.5346	-1034.5326	-1034.5507	0.00	39.43	40.68	29.36	1.23	40.66	41.91	30.59

ACN-NQP-PhOH-S0-02-1-6311

ACN-NQP-PhOH-T1-02-1-6311

ACN-NQP-PhOH-T1-TS-02-1-6311

ACN-NQP-PhOH-T1-02-1-prod-6311

					Relative to ACN-NQP-PhOH-S0-02-2-6311				Relative to ACN-NQP-PhOH-S0-01-2-6311			
Total Electronic Energy=	-1034.855	-1034.7878	-1034.7842	-1034.8052	0.00	42.16	44.39	31.19	0.16	42.33	44.55	31.36
Zero-point correction=	0.309111	0.306688	0.302622	0.306905	0.00	-1.52	-4.07	-1.38	0.16	-1.36	-3.92	-1.23
Thermal correction to Energy=	0.328477	0.32618	0.321442	0.326273	0.00	-1.44	-4.41	-1.38	0.07	-1.37	-4.34	-1.31
Thermal correction to Enthalpy=	0.329422	0.327124	0.322386	0.327217	0.00	-1.44	-4.42	-1.38	0.07	-1.37	-4.34	-1.31
Thermal correction to Gibbs Free Energy=	0.257604	0.253624	0.25156	0.254748	0.00	-2.50	-3.79	-1.79	1.13	-1.37	-2.66	-0.66
Sum of electronic and zero-point Energies=	-1034.5458	-1034.4811	-1034.4816	-1034.4983	0.00	40.64	40.32	29.81	0.32	40.96	40.64	30.13
Sum of electronic and thermal Energies=	-1034.5265	-1034.4616	-1034.4628	-1034.479	0.00	40.72	39.97	29.81	0.23	40.96	40.21	30.05
Sum of electronic and thermal Enthalpies=	-1034.5255	-1034.4606	-1034.4618	-1034.478	0.00	40.72	39.97	29.81	0.24	40.96	40.21	30.05
Sum of electronic and thermal Free Energies=	-1034.5973	-1034.5341	-1034.5327	-1034.5505	0.00	39.67	40.60	29.40	1.30	40.96	41.89	30.70

ACN-NQP-PhOH-S0-02-2-6311

ACN-NQP-PhOH-T1-02-2-6311

ACN-NQP-PhOH-T1-TS-02-2-6311

ACN-NQP-PhOH-T1-02-2-prod-6311

Hydrogen abstraction NQF-Indole

B3LYP/6-31+Gd	So	T1-complex	T1-TS	T1-RP	So	T1-complex	T1-TS	T1-RP
Imaginary Vibration (cm^{-1})			-1001.13					
Total Electronic Energy =	-1051.636955	-1051.584367	-1051.581145	-1051.58387	0.00	33.00	35.02	33.31
Zero-point correction=	0.303385	0.301126	0.29668	0.300438	0.00	-1.42	-4.21	-1.85
Thermal correction to Energy=	0.323201	0.320473	0.315695	0.319892	0.00	-1.71	-4.71	-2.08
Thermal correction to Enthalpy=	0.324145	0.321417	0.316639	0.320836	0.00	-1.71	-4.71	-2.08
Thermal correction to Gibbs Free Energy=	0.24884	0.248022	0.245221	0.247602	0.00	-0.51	-2.27	-0.78
Sum of electronic and zero-point Energies=	-1051.33357	-1051.283241	-1051.284464	-1051.283432	0.00	31.58	30.81	31.46
Sum of electronic and thermal Energies=	-1051.313754	-1051.263894	-1051.26545	-1051.263978	0.00	31.29	30.31	31.23
Sum of electronic and thermal Enthalpies=	-1051.31281	-1051.26295	-1051.264506	-1051.263034	0.00	31.29	30.31	31.23
Sum of electronic and thermal Free Energies=	-1051.388115	-1051.336346	-1051.335924	-1051.336268	0.00	32.49	32.75	32.53
	ACN-NQF-indole-S0-631+Gdp							
		ACN-NQF-indole-T1-631+Gdp						
			ACN-NQF-indole-T1-TS02-631+Gd					
				ACN-NQF-indole-T1-prod-631+Gdp				

B3LYP/6-311++Gdp/6-31+Gd frequency from 6-31+Gd calculation	So	T1-complex	T1-TS	T1-RP	So	T1-complex	T1-TS	T1-RP
Total Electronic Energy =	-1051.875548	-1051.821696	-1051.819929	-1051.822739	0.00	33.79	34.90	33.14
Zero-point correction=	0.303385	0.301126	0.29668	0.300438	0.00	-1.42	-4.21	-1.85
Thermal correction to Energy=	0.323201	0.320473	0.315695	0.319892	0.00	-1.71	-4.71	-2.08
Thermal correction to Enthalpy=	0.324145	0.321417	0.316639	0.320836	0.00	-1.71	-4.71	-2.08
Thermal correction to Gibbs Free Energy=	0.24884	0.248022	0.245221	0.247602	0.00	-0.51	-2.27	-0.78
Sum of electronic and zero-point Energies=	-1051.572163	-1051.52057	-1051.523249	-1051.522301	0.00	32.37	30.69	31.29
Sum of electronic and thermal Energies=	-1051.552347	-1051.501223	-1051.504234	-1051.502847	0.00	32.08	30.19	31.06
Sum of electronic and thermal Enthalpies=	-1051.551403	-1051.500279	-1051.50329	-1051.501903	0.00	32.08	30.19	31.06
Sum of electronic and thermal Free Energies=	-1051.626708	-1051.573674	-1051.574708	-1051.575137	0.00	33.28	32.63	32.36
	ACN-NQF-indole-S0-6311++Gdp							
		ACN-NQF-indole-T1-6311++Gdp						
			ACN-NQF-indole-T1-TS02-6311++Gdp					
				ACN-NQF-indole-T1-prod-6311++Gdp				