Supporting Information

Computational Replication of the Abnormal Secondary Kinetic Isotope Effects in a Hydride Transfer Reaction in Solution with a Motion Assisted H-Tunneling Model

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Table S1. The atom coordinates and absolute energies of the TRS of DAD = 2.9 Å

H in Acceptor Well Total Energy = -770.136997442

O	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.83103195
C	1.18547483	0.00000000	0.66996381
C	-1.17817203	0.15885150	0.67166120
C	-1.22446023	0.22033631	2.08218740
C	1.24251319	0.05415584	2.08087470
C	-2.33416256	0.28740275	-0.10361984
H	-2.25880850	0.23138926	-1.18458327
C	-3.54964433	0.49473472	0.53579349
H	-4.45235064	0.59982139	-0.05821445
C	-2.47574597	0.44550592	2.70174635
H	-2.52166559	0.51237846	3.78605514
C	-3.62356785	0.58651434	1.94063860
H	-4.57918352	0.76672530	2.42270303
C	2.35094423	-0.02456158	-0.10542129
H	2.26788620	-0.06408959	-1.18670391
C	3.58336764	0.01666928	0.53305742
H	4.49167447	0.00615181	-0.06171304
C	2.51384251	0.10632471	2.70012444
H	2.56772217	0.17221728	3.78430941
C	3.67013164	0.09227911	1.93887017
H	4.64163221	0.14516613	2.42015603
C	-0.13121880	-2.85288203	3.33483605
O	0.11486142	-3.00193567	2.01086094
H	1.06088853	-3.14166632	1.82922013
C	0.95977021	-3.19001487	4.30957394
H	1.02969587	-4.28355774	4.40894871
H	0.73682989	-2.78009948	5.29855717
H	1.93362908	-2.81062047	3.98110408
H	-0.05452367	-1.18542312	3.04037155
H	0.02046936	0.37201674	3.85439020
C	-1.56395899	-3.10578239	3.69384160
H	-1.79935661	-2.69337562	4.67847152
H	-1.73110000	-4.19252767	3.72780396
H	-2.23812719	-2.68366524	2.94411174

H in Donor Well Total Energy = -770.136997442

O	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.83103195
C	1.18547483	0.00000000	0.66996381
C	-1.17817203	0.15885150	0.67166120
C	-1.22446023	0.22033631	2.08218740
C	1.24251319	0.05415584	2.08087470
C	-2.33416256	0.28740275	-0.10361984
H	-2.25880850	0.23138926	-1.18458327
C	-3.54964433	0.49473472	0.53579349
H	-4.45235064	0.59982139	-0.05821445
C	-2.47574597	0.44550592	2.70174635
H	-2.52166559	0.51237846	3.78605514
C	-3.62356785	0.58651434	1.94063860
H	-4.57918352	0.76672530	2.42270303
C	2.35094423	-0.02456158	-0.10542129
H	2.26788620	-0.06408959	-1.18670391
C	3.58336764	0.01666928	0.53305742
H	4.49167447	0.00615181	-0.06171304
C	2.51384251	0.10632471	2.70012444
H	2.56772217	0.17221728	3.78430941
C	3.67013164	0.09227911	1.93887017
H	4.64163221	0.14516613	2.42015603
C	-0.13121880	-2.85288203	3.33483605
O	0.11486142	-3.00193567	2.01086094
H	1.06088853	-3.14166632	1.82922013
C	0.95977021	-3.19001487	4.30957394
H	1.02969587	-4.28355774	4.40894871
H	0.73682989	-2.78009948	5.29855717
H	1.93362908	-2.81062047	3.98110408
H	-0.07669499	-1.66745843	3.12549647
H	0.02046936	0.37201674	3.85439020
C	-1.56395899	-3.10578239	3.69384160
H	-1.79935661	-2.69337562	4.67847152
H	-1.73110000	-4.19252767	3.72780396
H	-2.23812719	-2.68366524	2.94411174

H at the Midpoint Total Energy = -770.136700

O	-0.33332941	2.08752452	-0.98798867
C	0.12520546	0.21399343	1.08430031
C	0.94463779	1.79493565	-0.62002594
C	-1.39072446	1.61054037	-0.26767156
C	-1.20944957	0.71661615	0.81100784
C	1.22808661	0.90848431	0.44332711
C	-2.65984530	2.07155379	-0.62919922
H	-2.75920411	2.75511797	-1.46595925
C	-3.76046888	1.64698394	0.10401509
H	-4.74978721	2.00291308	-0.16678538
C	-2.34905047	0.31381061	1.54539963
H	-2.22038198	-0.36020070	2.38888121
C	-3.60812574	0.77568707	1.20179217
H	-4.47720912	0.46826321	1.77472326
C	1.96937844	2.43816405	-1.32451954
H	1.71328856	3.11397070	-2.13404928
C	3.28753976	2.20284547	-0.95668626
H	4.08749907	2.70421331	-1.49295215
C	2.58124299	0.69892100	0.80043266
H	2.80836635	0.03696122	1.63285560
C	3.59895584	1.33939963	0.11431277
H	4.63397178	1.18353350	0.40188213
C	0.14796605	-2.24389368	-0.45461467
O	0.17996904	-1.44653401	-1.54954795
H	1.08725032	-1.30923723	-1.87432025
C	1.39043151	-2.99927787	-0.08084010
H	1.50257195	-3.86408809	-0.75175790
H	1.32054188	-3.37927032	0.94216723
H	2.28853903	-2.37772822	-0.16636442
H	0.13658583	-1.01494965	0.31484314
H	0.30194175	-0.18578877	2.08180618
C	-1.20100655	-2.85055991	-0.21415562
H	-1.28395188	-3.22741514	0.80862961
H	-1.33349211	-3.69721185	-0.90389090
H	-1.99794320	-2.12827755	-0.40904676

Table S2. The atom coordinates and absolute energies of the TRS of DAD = 3.0 Å

H in Acceptor Well Total Energy = -770.135362027

O	-0.33264839	2.12267087	-0.96227652
C	0.12426637	0.22972214	1.09416748
C	0.94481563	1.82588465	-0.59729118
C	-1.38946666	1.64304146	-0.24436933
C	-1.20927337	0.73361464	0.82192534
C	1.22736112	0.92313345	0.45272331
C	-2.65547099	2.12250016	-0.59226257
H	-2.75117709	2.82198770	-1.41638034
C	-3.75605474	1.70077975	0.14240836
H	-4.74311780	2.07276990	-0.11600428
C	-2.34968908	0.33084215	1.55550119
H	-2.22348555	-0.35604346	2.38884050
C	-3.60576567	0.81048961	1.22560801
H	-4.47477225	0.50520343	1.79991513
C	1.96806504	2.48413152	-1.28952629
H	1.71026254	3.17633414	-2.08469390
C	3.28644233	2.24618824	-0.92468278
H	4.08583033	2.75982464	-1.45075430
C	2.58121851	0.70816308	0.80428930
H	2.80969836	0.03090743	1.62394584
C	3.59814108	1.36157189	0.12912543
H	4.63352514	1.20145960	0.41321331
C	0.14781178	-2.31292075	-0.49781416
O	0.17981477	-1.51556139	-1.59274699
H	1.08829446	-1.36860264	-1.91032453
C	1.39021047	-3.07034904	-0.13080927
H	1.50431723	-3.92415252	-0.81578530
H	1.32013453	-3.46656492	0.88563724
H	2.28743939	-2.44647190	-0.20786962
H	0.13372384	-0.79157317	0.45472127
H	0.30100255	-0.17005992	2.09167301
C	-1.20429403	-2.91123959	-0.25673350
H	-1.28216110	-3.30899188	0.75817470
H	-1.35179127	-3.74127366	-0.96357686
H	-1.99552281	-2.17738931	-0.43142308

H in Donor Well Total Energy = -770.135664252

O	-0.33264839	2.12267087	-0.96227652
C	0.12426637	0.22972214	1.09416748
C	0.94481563	1.82588465	-0.59729118
C	-1.38946666	1.64304146	-0.24436933
C	-1.20927337	0.73361464	0.82192534
C	1.22736112	0.92313345	0.45272331
C	-2.65547099	2.12250016	-0.59226257
H	-2.75117709	2.82198770	-1.41638034
C	-3.75605474	1.70077975	0.14240836
H	-4.74311780	2.07276990	-0.11600428
C	-2.34968908	0.33084215	1.55550119
H	-2.22348555	-0.35604346	2.38884050
C	-3.60576567	0.81048961	1.22560801
H	-4.47477225	0.50520343	1.79991513
C	1.96806504	2.48413152	-1.28952629
H	1.71026254	3.17633414	-2.08469390
C	3.28644233	2.24618824	-0.92468278
H	4.08583033	2.75982464	-1.45075430
C	2.58121851	0.70816308	0.80428930
H	2.80969836	0.03090743	1.62394584
C	3.59814108	1.36157189	0.12912543
H	4.63352514	1.20145960	0.41321331
C	0.14781178	-2.31292075	-0.49781416
O	0.17981477	-1.51556139	-1.59274699
H	1.08829446	-1.36860264	-1.91032453
C	1.39021047	-3.07034904	-0.13080927
H	1.50431723	-3.92415252	-0.81578530
H	1.32013453	-3.46656492	0.88563724
H	2.28743939	-2.44647190	-0.20786962
H	0.13835446	-1.29162545	0.14163207
H	0.30100255	-0.17005992	2.09167301
C	-1.20429403	-2.91123959	-0.25673350
H	-1.28216110	-3.30899188	0.75817470
H	-1.35179127	-3.74127366	-0.96357686
H	-1.99552281	-2.17738931	-0.43142308

H at the Midpoint Total Energy= -770.133113

O	-0.33264839	2.12267087	-0.96227652
C	0.12426637	0.22972214	1.09416748
C	0.94481563	1.82588465	-0.59729118
C	-1.38946666	1.64304146	-0.24436933
C	-1.20927337	0.73361464	0.82192534
C	1.22736112	0.92313345	0.45272331
C	-2.65547099	2.12250016	-0.59226257
H	-2.75117709	2.82198770	-1.41638034
C	-3.75605474	1.70077975	0.14240836
H	-4.74311780	2.07276990	-0.11600428
C	-2.34968908	0.33084215	1.55550119
H	-2.22348555	-0.35604346	2.38884050
C	-3.60576567	0.81048961	1.22560801
H	-4.47477225	0.50520343	1.79991513
C	1.96806504	2.48413152	-1.28952629
H	1.71026254	3.17633414	-2.08469390
C	3.28644233	2.24618824	-0.92468278
H	4.08583033	2.75982464	-1.45075430
C	2.58121851	0.70816308	0.80428930
H	2.80969836	0.03090743	1.62394584
C	3.59814108	1.36157189	0.12912543
H	4.63352514	1.20145960	0.41321331
C	0.14781178	-2.31292075	-0.49781416
O	0.17981477	-1.51556139	-1.59274699
H	1.08829446	-1.36860264	-1.91032453
C	1.39021047	-3.07034904	-0.13080927
H	1.50431723	-3.92415252	-0.81578530
H	1.32013453	-3.46656492	0.88563724
H	2.28743939	-2.44647190	-0.20786962
H	0.13603918	-1.04159930	0.29817669
H	0.30100255	-0.17005992	2.09167301
C	-1.20429403	-2.91123959	-0.25673350
H	-1.28216110	-3.30899188	0.75817470
H	-1.35179127	-3.74127366	-0.96357686
H	-1.99552281	-2.17738931	-0.43142308

Table S3. The atom coordinates and absolute energies of the TRS of DAD = 3.1 Å

H in Acceptor Well Total Energy= -770.133336821

O	-0.33359564	2.15109461	-0.94529927
C	0.12433496	0.26939874	1.11848949
C	0.94437125	1.85790931	-0.57845041
C	-1.39028260	1.67364764	-0.22598934
C	-1.20904772	0.76777021	0.84355704
C	1.22687500	0.95898479	0.47512536
C	-2.65673639	2.14987596	-0.57647520
H	-2.75312726	2.84651055	-1.40290940
C	-3.75697546	1.72832777	0.15872887
H	-4.74456756	2.09767249	-0.10147578
C	-2.34935205	0.36511718	1.57750215
H	-2.22245651	-0.31938935	2.41263903
C	-3.60584012	0.84129973	1.24476981
H	-4.47492382	0.53601887	1.81899183
C	1.96701577	2.51474126	-1.27259510
H	1.70900979	3.20365832	-2.07052428
C	3.28533330	2.27966314	-0.90573841
H	4.08462045	2.79223863	-1.43300147
C	2.58062105	0.74692164	0.82850693
H	2.80922605	0.07174048	1.64979006
C	3.59706785	1.39911160	0.15162616
H	4.63247575	1.24104716	0.43681765
C	0.14866525	-2.35799791	-0.52655761
O	0.18066813	-1.56063887	-1.62149005
H	1.09042279	-1.40675514	-1.93239537
C	1.39079680	-3.11151548	-0.15442455
H	1.50267064	-3.97147441	-0.83244226
H	1.32146497	-3.49927582	0.86524594
H	2.28871911	-2.48980622	-0.23788259
H	0.13379240	-0.75189656	0.47904327
H	0.30107104	-0.13038319	2.11599450
C	-1.20295271	-2.95340928	-0.28210576
H	-1.28417704	-3.33824932	0.73745175
H	-1.34615077	-3.79362679	-0.97822699
H	-1.99445196	-2.22352524	-0.47014115

H in Donor Well Total Energy= -770.134196286

O	-0.33359564	2.15109461	-0.94529927
C	0.12433496	0.26939874	1.11848949
C	0.94437125	1.85790931	-0.57845041
C	-1.39028260	1.67364764	-0.22598934
C	-1.20904772	0.76777021	0.84355704
C	1.22687500	0.95898479	0.47512536
C	-2.65673639	2.14987596	-0.57647520
H	-2.75312726	2.84651055	-1.40290940
C	-3.75697546	1.72832777	0.15872887
H	-4.74456756	2.09767249	-0.10147578
C	-2.34935205	0.36511718	1.57750215
H	-2.22245651	-0.31938935	2.41263903
C	-3.60584012	0.84129973	1.24476981
H	-4.47492382	0.53601887	1.81899183
C	1.96701577	2.51474126	-1.27259510
H	1.70900979	3.20365832	-2.07052428
C	3.28533330	2.27966314	-0.90573841
H	4.08462045	2.79223863	-1.43300147
C	2.58062105	0.74692164	0.82850693
H	2.80922605	0.07174048	1.64979006
C	3.59706785	1.39911160	0.15162616
H	4.63247575	1.24104716	0.43681765
C	0.14866525	-2.35799791	-0.52655761
O	0.18066813	-1.56063887	-1.62149005
H	1.09042279	-1.40675514	-1.93239537
C	1.39079680	-3.11151548	-0.15442455
H	1.50267064	-3.97147441	-0.83244226
H	1.32146497	-3.49927582	0.86524594
H	2.28871911	-2.48980622	-0.23788259
H	0.13920785	-1.33670300	0.11288838
H	0.30107104	-0.13038319	2.11599450
C	-1.20295271	-2.95340928	-0.28210576
H	-1.28417704	-3.33824932	0.73745175
H	-1.34615077	-3.79362679	-0.97822699
H	-1.99445196	-2.22352524	-0.47014115

H at the Midpoint Total Energy= -770.128696

O	-0.33351841	2.14274107	-0.95053043
C	0.12441237	0.26104444	1.11325913
C	0.94444897	1.84955564	-0.58368144
C	-1.39020576	1.66529393	-0.23122024
C	-1.20897085	0.75941614	0.83832659
C	1.22695286	0.95063076	0.46989478
C	-2.65666010	2.14152243	-0.58170623
H	-2.75305096	2.83815728	-1.40814074
C	-3.75689957	1.71997405	0.15349816
H	-4.74449208	2.08931896	-0.10670664
C	-2.34927563	0.35676293	1.57227197
H	-2.22238004	-0.32774387	2.40740921
C	-3.60576419	0.83294566	1.23953950
H	-4.47484824	0.52766472	1.81376179
C	1.96709395	2.50638786	-1.27782640
H	1.70908782	3.19530519	-2.07575589
C	3.28541197	2.27130965	-0.91096958
H	4.08469943	2.78388537	-1.43823281
C	2.58069944	0.73856752	0.82327648
H	2.80930454	0.06338609	1.64455993
C	3.59714665	1.39075775	0.14639544
H	4.63255495	1.23269327	0.43158702
C	0.14874266	-2.36635323	-0.53178859
O	0.18074559	-1.56899388	-1.62672148
H	1.09050060	-1.41511010	-1.93762694
C	1.39087470	-3.11987111	-0.15965540
H	1.50274859	-3.97983036	-0.83767338
H	1.32154288	-3.50763159	0.86001550
H	2.28879737	-2.49816159	-0.24311349
H	0.13657757	-1.05265439	0.29073529
H	0.30114854	-0.13873762	2.11076455
C	-1.20287584	-2.96176483	-0.28733665
H	-1.28410017	-3.34660504	0.73222126
H	-1.34607394	-3.80198270	-0.98345815
H	-1.99437540	-2.23188052	-0.47537213

Table S4. The atom coordinates and absolute energies of the TRS of DAD = 3.2 Å

H in Acceptor Well Total Energy = -770.131423157

O	-0.33379789	2.10827185	-0.97893863
C	0.12510449	0.29270941	1.14245920
C	0.94456112	1.83256824	-0.59903640
C	-1.39065471	1.65194074	-0.24634720
C	-1.20871428	0.77899728	0.85048058
C	1.22646388	0.96883055	0.48398680
C	-2.65727387	2.11571711	-0.61225492
H	-2.75375089	2.78686674	-1.45954721
C	-3.75757190	1.71553528	0.13475758
H	-4.74539885	2.07583441	-0.13698721
C	-2.34915377	0.39726484	1.59516608
H	-2.22253705	-0.26296844	2.44970191
C	-3.60596538	0.86162510	1.24704654
H	-4.47509627	0.57243446	1.82954320
C	1.96635525	2.47315932	-1.30913679
H	1.70806246	3.13500845	-2.12957260
C	3.28421875	2.25855533	-0.92798724
H	4.08322046	2.75916136	-1.46700215
C	2.57943849	0.77754887	0.85123127
H	2.80841700	0.12932827	1.69384098
C	3.59525949	1.41492341	0.15925736
H	4.63004476	1.27298860	0.45513676
C	0.15021955	-2.41944081	-0.55565319
O	0.18222254	-1.62208209	-1.65058515
H	1.09333924	-1.45805917	-1.95209377
C	1.39230379	-3.16817155	-0.17753837
H	1.50257142	-4.03468218	-0.84785115
H	1.32346034	-3.54658716	0.84555701
H	2.29060657	-2.54822260	-0.26752344
H	0.13456194	-0.72858550	0.50301326
H	0.29951320	-0.05378164	2.16010464
C	-1.20114488	-3.01041774	-0.30573955
H	-1.28405279	-3.38231262	0.71840180
H	-1.34243795	-3.86035009	-0.99090020
H	-1.99239420	-2.28360810	-0.50498963

H in Donor Well Total Energy = -770.131382876

O	-0.33379789	2.10827185	-0.97893863
C	0.12510449	0.29270941	1.14245920
C	0.94456112	1.83256824	-0.59903640
C	-1.39065471	1.65194074	-0.24634720
C	-1.20871428	0.77899728	0.85048058
C	1.22646388	0.96883055	0.48398680
C	-2.65727387	2.11571711	-0.61225492
H	-2.75375089	2.78686674	-1.45954721
C	-3.75757190	1.71553528	0.13475758
H	-4.74539885	2.07583441	-0.13698721
C	-2.34915377	0.39726484	1.59516608
H	-2.22253705	-0.26296844	2.44970191
C	-3.60596538	0.86162510	1.24704654
H	-4.47509627	0.57243446	1.82954320
C	1.96635525	2.47315932	-1.30913679
H	1.70806246	3.13500845	-2.12957260
C	3.28421875	2.25855533	-0.92798724
H	4.08322046	2.75916136	-1.46700215
C	2.57943849	0.77754887	0.85123127
H	2.80841700	0.12932827	1.69384098
C	3.59525949	1.41492341	0.15925736
H	4.63004476	1.27298860	0.45513676
C	0.15021955	-2.41944081	-0.55565319
O	0.18222254	-1.62208209	-1.65058515
H	1.09333924	-1.45805917	-1.95209377
C	1.39230379	-3.16817155	-0.17753837
H	1.50257142	-4.03468218	-0.84785115
H	1.32346034	-3.54658716	0.84555701
H	2.29060657	-2.54822260	-0.26752344
H	0.14076218	-1.39814552	0.08379304
H	0.29951320	-0.05378164	2.16010464
C	-1.20114488	-3.01041774	-0.30573955
H	-1.28405279	-3.38231262	0.71840180
H	-1.34243795	-3.86035009	-0.99090020
H	-1.99239420	-2.28360810	-0.50498963

H at the Midpoint Total Energy= -770.123005

O	-0.33388661	2.11783785	-0.97295018
C	0.12501595	0.30227469	1.14844850
C	0.94447294	1.84213409	-0.59304776
C	-1.39074383	1.66150656	-0.24035844
C	-1.20880336	0.78856274	0.85646975
C	1.22637579	0.97839610	0.48997583
C	-2.65736348	2.12528310	-0.60626634
H	-2.75384055	2.79643300	-1.45355894
C	-3.75766196	1.72510109	0.14074648
H	-4.74548931	2.08540035	-0.13099840
C	-2.34924330	0.40683011	1.60115556
H	-2.22262653	-0.25340339	2.45569175
C	-3.60605539	0.87119060	1.25303589
H	-4.47518665	0.58199982	1.83553276
C	1.96626748	2.48272544	-1.30314847
H	1.70797454	3.14457484	-2.12358460
C	3.28413147	2.26812136	-0.92199874
H	4.08313349	2.76872757	-1.46101388
C	2.57935094	0.78711433	0.85722044
H	2.80832953	0.13889346	1.69983051
C	3.59517234	1.42448908	0.16524626
H	4.62995801	1.28255423	0.46112579
C	0.15013106	-2.40987666	-0.54966456
O	0.18213404	-1.61251763	-1.64459697
H	1.09325111	-1.44849461	-1.94610567
C	1.39221579	-3.15860766	-0.17154960
H	1.50248347	-4.02511865	-0.84186266
H	1.32337230	-3.53702346	0.85154618
H	2.29051894	-2.53865850	-0.26153467
H	0.13757358	-1.05380043	0.29939236
H	0.29942475	-0.04421655	2.16609434
C	-1.20123396	-3.00085381	-0.29975083
H	-1.28414187	-3.37274882	0.72439092
H	-1.34252708	-3.85078647	-0.98491175
H	-1.99248359	-2.27404386	-0.49900100

Table S5. The atom coordinates and absolute energies of the TRS of DAD = 3.3 Å

H in Acceptor Well Total Energy = -770.129220629

O	-0.33359596	2.11444947	-0.97682223
C	0.12475253	0.32479532	1.16289480
C	0.94491762	1.84842841	-0.58999911
C	-1.39093364	1.66519319	-0.24075163
C	-1.20889177	0.80196886	0.86403101
C	1.22588999	0.99492570	0.50149277
C	-2.65769113	2.12341531	-0.61253618
H	-2.75441109	2.78705301	-1.46568038
C	-3.75820850	1.72749124	0.13659266
H	-4.74632655	2.08386541	-0.13934724
C	-2.34977640	0.42397103	1.61013348
H	-2.22309782	-0.23028927	2.46917753
C	-3.60675078	0.88283515	1.25607615
H	-4.47639202	0.59646031	1.83917475
C	1.96655200	2.48643399	-1.30212096
H	1.70902318	3.14017163	-2.12926716
C	3.28382097	2.28033027	-0.91372650
H	4.08299302	2.77944450	-1.45390904
C	2.57813164	0.81239852	0.87591918
H	2.80625044	0.17172001	1.72442519
C	3.59393178	1.44773704	0.18229329
H	4.62814756	1.31251897	0.48321087
C	0.15065252	-2.47210742	-0.58828230
O	0.18265540	-1.67474965	-1.68321289
H	1.09482803	-1.50185434	-1.97662478
C	1.39354942	-3.21425546	-0.20290024
H	1.50515481	-4.08681633	-0.86550143
H	1.32447181	-3.58359796	0.82338968
H	2.29100811	-2.59407791	-0.29795541
H	0.13421004	-0.69649959	0.52344886
H	0.29872658	-0.01271724	2.18362603
C	-1.19976315	-3.06080126	-0.33497235
H	-1.28497737	-3.42035706	0.69326992
H	-1.33776897	-3.91982779	-1.00979917
H	-1.99108205	-2.33765613	-0.54574716

H in Donor Well Total Energy = -770.129709544

O	-0.33359596	2.11444947	-0.97682223
C	0.12475253	0.32479532	1.16289480
C	0.94491762	1.84842841	-0.58999911
C	-1.39093364	1.66519319	-0.24075163
C	-1.20889177	0.80196886	0.86403101
C	1.22588999	0.99492570	0.50149277
C	-2.65769113	2.12341531	-0.61253618
H	-2.75441109	2.78705301	-1.46568038
C	-3.75820850	1.72749124	0.13659266
H	-4.74632655	2.08386541	-0.13934724
C	-2.34977640	0.42397103	1.61013348
H	-2.22309782	-0.23028927	2.46917753
C	-3.60675078	0.88283515	1.25607615
H	-4.47639202	0.59646031	1.83917475
C	1.96655200	2.48643399	-1.30212096
H	1.70902318	3.14017163	-2.12926716
C	3.28382097	2.28033027	-0.91372650
H	4.08299302	2.77944450	-1.45390904
C	2.57813164	0.81239852	0.87591918
H	2.80625044	0.17172001	1.72442519
C	3.59393178	1.44773704	0.18229329
H	4.62814756	1.31251897	0.48321087
C	0.15065252	-2.47210742	-0.58828230
O	0.18265540	-1.67474965	-1.68321289
H	1.09482803	-1.50185434	-1.97662478
C	1.39354942	-3.21425546	-0.20290024
H	1.50515481	-4.08681633	-0.86550143
H	1.32447181	-3.58359796	0.82338968
H	2.29100811	-2.59407791	-0.29795541
H	0.14119512	-1.45081214	0.05116395
H	0.29872658	-0.01271724	2.18362603
C	-1.19976315	-3.06080126	-0.33497235
H	-1.28497737	-3.42035706	0.69326992
H	-1.33776897	-3.91982779	-1.00979917
H	-1.99108205	-2.33765613	-0.54574716

H at the Midpoint Total Energy = -770.117623

O	-0.33369586	2.12522621	-0.97007570
C	0.12465278	0.33557137	1.16964218
C	0.94481819	1.85920505	-0.58325242
C	-1.39103398	1.67596977	-0.23400478
C	-1.20899205	0.81274507	0.87077828
C	1.22579066	1.00570202	0.50823988
C	-2.65779199	2.13419206	-0.60578949
H	-2.75451201	2.79783002	-1.45893406
C	-3.75830978	1.73826783	0.14333967
H	-4.74642825	2.09464216	-0.13260039
C	-2.34987716	0.43474709	1.61688107
H	-2.22319852	-0.21951348	2.47592543
C	-3.60685201	0.89361142	1.26282359
H	-4.47649362	0.60723647	1.84592239
C	1.96645299	2.49721089	-1.29537454
H	1.70892406	3.15094880	-2.12252111
C	3.28372249	2.29110707	-0.90697991
H	4.08289486	2.79022151	-1.44716267
C	2.57803289	0.82317473	0.88266645
H	2.80615175	0.18249596	1.73117283
C	3.59383341	1.45851352	0.18904029
H	4.62804961	1.32329540	0.48995798
C	0.15055277	-2.46133248	-0.58153561
O	0.18255571	-1.66397439	-1.67646662
H	1.09472865	-1.49107902	-1.96987862
C	1.39345020	-3.20348084	-0.19615339
H	1.50505559	-4.07604207	-0.85875485
H	1.32437254	-3.57282349	0.83013695
H	2.29090921	-2.58330302	-0.29120861
H	0.13760291	-1.06288060	0.29405341
H	0.29862688	-0.00194134	2.19037383
C	-1.19986342	-3.05002658	-0.32822555
H	-1.28507770	-3.40958254	0.70001713
H	-1.33786930	-3.90905343	-1.00305264
H	-1.99118265	-2.32688113	-0.53900047

Table S6. The atom coordinates and absolute energies of the TRS of DAD = 3.5 Å

H in Acceptor Well Total Energy= -770.126144248

O	-0.33554746	2.18501856	-0.93303966
C	0.12339578	0.36196011	1.17546641
C	0.94324976	1.91010744	-0.55336127
C	-1.39206709	1.72443260	-0.20370675
C	-1.20937702	0.83321973	0.87834196
C	1.22383430	1.02973073	0.51618463
C	-2.65675708	2.20413757	-0.55359893
H	-2.75210113	2.89296875	-1.38624233
C	-3.75533486	1.79882087	0.19308315
H	-4.74167677	2.17461240	-0.06248178
C	-2.34896395	0.44342861	1.62130854
H	-2.22129317	-0.23648493	2.46028264
C	-3.60417475	0.92027877	1.28659591
H	-4.47242658	0.62441176	1.86704968
C	1.96385478	2.56883855	-1.24668310
H	1.70505858	3.24508246	-2.05470596
C	3.28103215	2.35533964	-0.86240268
H	4.07984299	2.87304507	-1.38533775
C	2.57641605	0.83794089	0.88598699
H	2.80405309	0.17184749	1.71509892
C	3.59178280	1.49119999	0.20893756
H	4.62607233	1.34749212	0.50572074
C	0.15086541	-2.60445211	-0.68184276
O	0.18286834	-1.80709461	-1.77677303
H	1.09684112	-1.60248857	-2.04360891
C	1.39611037	-3.32648227	-0.27356151
H	1.52014968	-4.21115007	-0.91832235
H	1.32273484	-3.67585807	0.75923189
H	2.28863497	-2.70049822	-0.37289497
H	0.13285328	-0.65933480	0.53602046
H	0.29692177	0.03345140	2.19920648
C	-1.20003043	-3.17958802	-0.41421274
H	-1.28173648	-3.52489461	0.61897706
H	-1.34877517	-4.04675879	-1.07685633
H	-1.98631052	-2.45228048	-0.62785998

H in Donor Well Total Energy = -770.125287833

O	-0.33579172	2.21141259	-0.91651309
C	0.12315130	0.38835488	1.19199213
C	0.94300496	1.93650157	-0.53683486
C	-1.39231093	1.75082684	-0.18718050
C	-1.20962097	0.85961428	0.89486779
C	1.22358940	1.05612524	0.53271062
C	-2.65700045	2.23053159	-0.53707252
H	-2.75234444	2.91936251	-1.36971560
C	-3.75557780	1.82521506	0.20960925
H	-4.74191930	2.20100643	-0.04595559
C	-2.34920743	0.46982332	1.63783410
H	-2.22153670	-0.21008995	2.47680783
C	-3.60441775	0.94667333	1.30312158
H	-4.47266920	0.65080642	1.88357513
C	1.96360956	2.59523242	-1.23015643
H	1.70481347	3.27147606	-2.03817897
C	3.28078640	2.38173361	-0.84587616
H	4.07959692	2.89943883	-1.36881103
C	2.57617061	0.86433544	0.90251281
H	2.80380755	0.19824231	1.73162443
C	3.59153694	1.51759428	0.22546366
H	4.62582606	1.37388647	0.52224672
C	0.15062093	-2.57805618	-0.66531630
O	0.18262386	-1.78069899	-1.76024614
H	1.09659627	-1.57609301	-2.02708191
C	1.39586541	-3.30008602	-0.25703520
H	1.51990467	-4.18475350	-0.90179578
H	1.32248988	-3.64946172	0.77575777
H	2.28838964	-2.67410223	-0.35636861
H	0.14116358	-1.55676127	-0.02587030
H	0.29667723	0.05984627	2.21573178
C	-1.20027438	-3.15319182	-0.39768639
H	-1.28198038	-3.49849830	0.63550299
H	-1.34901906	-4.02036227	-1.06032971
H	-1.98655415	-2.42588460	-0.61133357

H at the Midpoint Total Energy = -770.106697

O	-0.33566980	2.19821687	-0.92477693
C	0.12327359	0.37515768	1.18372993
C	0.94312795	1.92330564	-0.54509844
C	-1.39218986	1.73763070	-0.19544376
C	-1.20949974	0.84641745	0.88660538
C	1.22371259	1.04292857	0.52444789
C	-2.65688032	2.21733588	-0.54533609
H	-2.75222443	2.90616732	-1.37797981
C	-3.75545858	1.81201902	0.20134631
H	-4.74180087	2.18781071	-0.05421874
C	-2.34908709	0.45662623	1.62957227
H	-2.22141625	-0.22328763	2.46854669
C	-3.60429842	0.93347655	1.29485949
H	-4.47255056	0.63760944	1.87531352
C	1.96373334	2.58203702	-1.23842053
H	1.70493703	3.25828119	-2.04644371
C	3.28091124	2.36853800	-0.85413995
H	4.07972239	2.88624365	-1.37707524
C	2.57629486	0.85113861	0.89425040
H	2.80393201	0.18504496	1.72336266
C	3.59166204	1.50439798	0.21720071
H	4.62595195	1.36069006	0.51398400
C	0.15074328	-2.59125571	-0.67357998
O	0.18274621	-1.79389788	-1.76851067
H	1.09671936	-1.58929179	-2.03534665
C	1.39598871	-3.31328618	-0.26529857
H	1.52002807	-4.19795435	-0.91005962
H	1.32261313	-3.66266215	0.76749525
H	2.28851368	-2.68730187	-0.36463203
H	0.13700859	-1.10804740	0.25507614
H	0.29679968	0.04664881	2.20747043
C	-1.20015310	-3.16639187	-0.40594986
H	-1.28185920	-3.51169857	0.62724037
H	-1.34889794	-4.03356297	-1.06859371
H	-1.98643350	-2.43908402	-0.61959715