Supporting Information

Computational Replication of the Primary Isotope Dependence of Secondary Kinetic Isotope Effects in Solution Hydride Transfer Reactions: Supporting the Isotopically Different Tunneling Ready State Conformations

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The TRS structures of the TXn^+ and $PhTXn^+$ reactions

The TRS structure of the reactions of the TXn^+ and $PhTXn^+$ at DAD = 3.1 Å and the corresponding degenerate double potential wells are shown in Figure S1. The TRS structure of the Xn^+ reaction has been reported by us and is also presented in this paper for comparison with the reaction of $PhXn^+$ (Figure 3 vs. Figure 1B in the paper).[1]

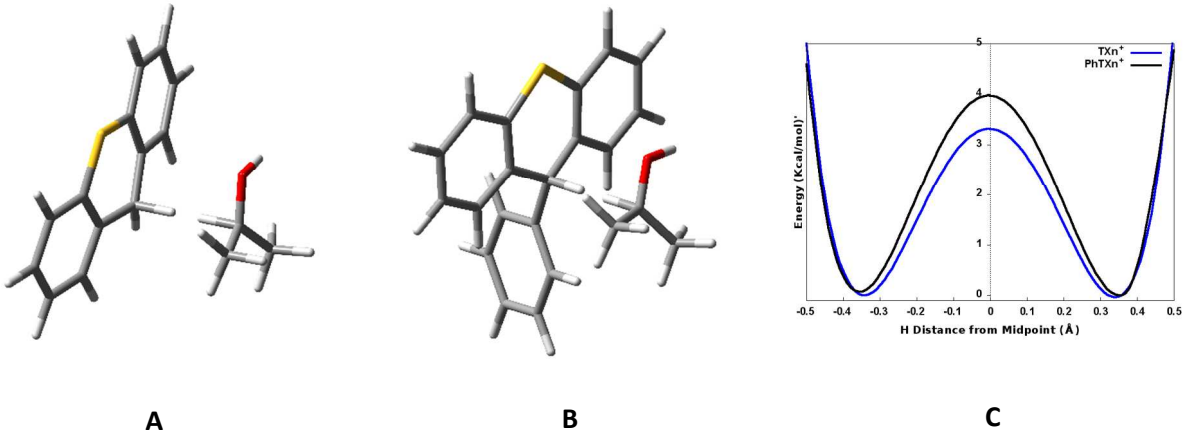

Figure S1. (**A**) The TRS structure with DAD = 3.1 Å for the reaction of the TXn^+ (left potential well for the Acceptor-H vibrations in the product TXnH; right for the Donor-H vibrations in the reactant 2-propanol). (**B**) The TRS structure with DAD = 3.1 Å for the reaction of the $PhTXn^+$ (left for the Acceptor-H vibrations in the product PhTXnH; right for Donor-H vibrations in the reactant 2-propanol). Although the transferring hydride is shown in both the donor and acceptor positions (i.e., in $(Donor\text{-}H)^{TRS}$ and $(Acceptor\text{-}H)^{TRS}$), it is indeed delocalized between the two. (**C**) The double-potential wells for the respective TRS's.

The observed KIEs do not fit to the calculated classical 2^o KIEs

The results inconsistent with the traditional TS theory are mainly the observed 1^o isotope dependence of 2^o KIEs. They cannot be fitted to the classical theory that assumes a same TS geometry for both the 1^o H- and D-transfers (although the C-H bond vibrational amplitude is a little larger than that of C-D bond!). Even so, it is interesting to know the classical 2^o KIEs calculated from the same method as used in the calculation of the tunneling ready states (TRSs) in the paper. Table S1 lists such TS geometry parameters and the 2^o KIEs and corresponding equilibrium isotope effects (EIEs). The bond-lengths and the acceptor ($PhXn^+$ and Xn^+) hybridizations in the TSs definitely suggest a late TS, which follows the Hammond's Postulate for an endothermic rate-limiting step, but the donor (2-

propanol) hybridization is only a little over halfway toward the formation of the product. This may be ONE reason that the calculated/observed β-D_6 2^o KIE on 2-propanol is not close to the calculated 2^o EIE (the Hammond's Postulate predicts 2^o KIE is closer to the EIE as compared to unity). Furthermore, the 9-α-D 2^o KIE on Xn^+ is 1.02 which is close to the small range from 1 to EIE (0.99). The calculated classical results are not consistent with the observed 2^o KIEs, *e.g.*, 1.02 for the β-2^o KIE on 2-propanol vs. the observed 1.05 for H-transfer and 1.00 for D-transfer; and 1.02 for the α-2^o KIE on Xn^+ vs. 0.99 and 0.98 for H- and D-transfers, respectively. We note that the magnitudes of the calculated 2^o KIEs for the TSs are not far from the observed ones. While different KIE values for the classical TSs may be given using other methods, in our work using the B3LYP/6-31+G* method, the calculations on the TRSs following the activated H-tunneling model agree very well with the observations, both the magnitude of the 2^o KIEs and the 1^o isotope dependence of 2^o KIEs.

Table S1. Parameters for the classical TS geometry and the calculated KIEs and EIEs (donor = 2-propanol, acceptor = Xn^+ and $PhXn^+$) [a]

	2-propanol/Xn^+	2-propanol/$PhXn^+$
Donor-Acceptor Distance (DAD)	2.77 Å	2.76 Å
Donor-H bond length (D-H)	1.62 Å	1.59 Å
Acceptor-H bond length (A-H)	1.19 Å	1.22 Å
Hybridization on donor C_D	$sp^{2.44}$	$sp^{2.50}$
Hybridization on acceptor C_A	$sp^{2.82}$	$sp^{2.79}$
β-2^o KIE (EIE) on donor	1.04 (1.22)	1.02 (1.25)
α-2^o KIE (EIE) on acceptor	1.02 (0.99)	N/A

[a] B3LYP/6-31+G* method

Table S2. The Relative energies of the double potential wells for the reactions of 2-propanol (donor) with various carbocations (acceptors) (for Table 1 data in the paper)

$PhXn^+$ Reaction	Energy in Hartree		
DAD	Donor well	Mid point	Acceptor well
2.9	-1001.19035022	-1001.18955541	-1001.19060141
3.0	-1001.18851190	-1001.18569654	-1001.18878705
3.1	-1001.18675766	-1001.18101627	-1001.18679738

3.2	-1001.18461956	-1001.17563215	-1001.18473370
3.3	-1001.18279958	-1001.17015870	-1001.18272089
3.5	-1001.17903071	-1001.15940742	-1001.17911154

$PhTXn^+$ Reaction	Energy in Hartree		
DAD	Donor well	Mid point	Acceptor well
2.8	-1324.15503972	-1324.15492613	-1324.15488274
2.9	-1324.15312463	-1324.15193480	-1324.15297447
3.0	-1324.15174851	-1324.14825663	-1324.15137378
3.1	-1324.15032218	-1324.14377177	-1324.14971169
3.2	-1324.14768111	-1324.13811796	-1324.14795498
3.3	-1324.14693412	-1324.13323190	-1324.14640487
3.5	-1324.14334430	-1324.12251805	-1324.14346058

TXn^+ Reaction	Energy in Hartree		
DAD	Donor well	Mid point	Acceptor well
2.9	-1093.10658831	-1093.10593172	-1093.10666143
3.0	-1093.10427796	-1093.10167395	-1093.10427735
3.1	-1093.10190816	-1093.09662916	-1093.10197109
3.2	-1093.10025702	-1093.09149325	-1093.09990303
3.3	-1093.09795002	-1093.08570278	-1093.09779613
3.5	-1093.09322662	-1093.07379688	-1093.09367099

Table S3. The atom coordinates and absolute energies of the TRS at different DADs for the reaction of $PhXn^+$ (for Table 1 data in the paper)

DAD=2.9 Å

H in Acceptor Well Total Energy = -1001.19060141

H	-2.38087	-3.99944	0.66516
C	-2.45195	-2.93953	0.44294
C	-2.56228	-0.19981	-0.15225
C	-1.28174	-2.23199	0.13535
C	-3.66502	-2.26817	0.45161

C	-3.72231	-0.89036	0.15451
C	-1.30467	-0.85485	-0.17877
H	-4.57651	-2.81056	0.68522
H	-4.67706	-0.37345	0.15961
H	-2.60569	0.85875	-0.38924
H	2.02414	-4.27281	-0.02812
C	2.15496	-3.22518	-0.27958
C	2.40757	-0.51479	-0.95478
C	3.38219	-2.71284	-0.67545
C	1.05007	-2.36984	-0.21617
C	1.14422	-0.9982	-0.5391
C	3.50797	-1.35382	-1.0209
H	4.24496	-3.37002	-0.73133
H	4.46689	-0.96395	-1.34814
H	2.50623	0.52793	-1.23686
C	0.22058	0.70579	2.35099
H	0.06939	0.22735	0.77913
C	-0.56953	1.9571	2.60314
H	-0.69149	2.08158	3.68993
H	-1.56492	1.91032	2.14919
H	-0.05191	2.84029	2.22297
C	1.68809	0.65742	2.65238
H	2.21086	1.51529	2.22239
H	2.1364	-0.26979	2.28561
H	1.8205	0.68683	3.74386
O	-0.39461	-0.48573	2.57423
H	-1.35472	-0.38673	2.69773
C	-0.04516	-0.1351	-0.41167
O	-0.13183	-2.95092	0.14142
C	-0.08887	1.11376	-1.2493
C	-0.09989	3.3594	-2.9464
C	0.55488	2.29981	-0.87071
C	-0.73269	1.06385	-2.49796
C	-0.73454	2.17789	-3.33914
C	0.54609	3.41704	-1.70928
H	1.0701	2.35296	0.08368
H	-1.22142	0.14822	-2.81904
H	-1.23411	2.11942	-4.30201
H	1.04494	4.32973	-1.39537
H	-0.10724	4.22713	-3.59954

H in Donor WellTotal Energy = -1001.19035022

H	-2.38169	-4.00202	0.65669
C	-2.45277	-2.94211	0.43447
C	-2.5631	-0.20239	-0.16072
C	-1.28255	-2.23457	0.12689

C	-3.66583	-2.27075	0.44314
C	-3.72312	-0.89294	0.14604
C	-1.30549	-0.85742	-0.18724
H	-4.57733	-2.81313	0.67675
H	-4.67788	-0.37603	0.15114
H	-2.6065	0.85617	-0.39771
H	2.02333	-4.27539	-0.03659
C	2.15414	-3.22776	-0.28805
C	2.40675	-0.51737	-0.96324
C	3.38138	-2.71542	-0.68392
C	1.04925	-2.37242	-0.22464
C	1.14341	-1.00077	-0.54756
C	3.50715	-1.3564	-1.02937
H	4.24415	-3.3726	-0.7398
H	4.46608	-0.96652	-1.3566
H	2.50541	0.52535	-1.24532
C	0.21977	0.70321	2.34252
H	0.10523	0.34076	1.15172
C	-0.57034	1.95453	2.59467
H	-0.69231	2.079	3.68146
H	-1.56573	1.90774	2.14072
H	-0.05272	2.83772	2.2145
C	1.68727	0.65484	2.64391
H	2.21005	1.51272	2.21393
H	2.13559	-0.27237	2.27714
H	1.81968	0.68425	3.7354
O	-0.39542	-0.48831	2.56577
H	-1.35554	-0.38931	2.68926
C	-0.04597	-0.13768	-0.42014
O	-0.13265	-2.9535	0.13295
C	-0.08969	1.11118	-1.25777
C	-0.10071	3.35682	-2.95487
C	0.55407	2.29723	-0.87917
C	-0.7335	1.06127	-2.50643
C	-0.73535	2.17532	-3.34761
C	0.54528	3.41446	-1.71775
H	1.06928	2.35038	0.07521
H	-1.22224	0.14564	-2.82751
H	-1.23492	2.11684	-4.31048
H	1.04413	4.32715	-1.40383
H	-0.10806	4.22456	-3.60801

H at the Midpoint Total Energy = -1001.18955541

H	3.90871	-1.80095	-1.25934
C	2.86642	-2.0092	-1.03996
C	0.157	-2.47289	-0.47741
C	1.99668	-0.93598	-0.80257

C	2.37169	-3.3035	-0.99122
C	1.01022	-3.53875	-0.70667
C	0.62553	-1.13522	-0.52691
H	3.03874	-4.14002	-1.17791
H	0.63044	-4.55537	-0.67453
H	-0.89281	-2.65185	-0.26647
H	3.47496	2.64412	-1.14627
C	2.41366	2.63921	-0.91935
C	-0.3352	2.54597	-0.37068
C	1.67668	3.81141	-0.82933
C	1.76753	1.41382	-0.72611
C	0.38739	1.33114	-0.43813
C	0.29549	3.76474	-0.56056
H	2.16884	4.76744	-0.98155
H	-0.27864	4.68479	-0.51049
H	-1.40241	2.5146	-0.17926
C	0.17361	-0.2394	2.65977
H	-0.02867	-0.11313	1.22951
C	-0.77509	-1.24608	3.24303
H	-0.41072	-1.53393	4.24096
H	-0.84111	-2.14962	2.62796
H	-1.77724	-0.82897	3.36214
C	0.21884	1.16177	3.19027
H	-0.78235	1.59479	3.25556
H	0.85662	1.79826	2.57111
H	0.64862	1.13714	4.2024
O	1.39428	-0.68121	2.25632
H	1.44154	-1.65257	2.22306
C	-0.23094	0.01314	-0.20075
O	2.54599	0.30214	-0.86961
C	-1.70926	-0.11428	-0.44884
C	-4.45516	-0.25121	-1.05251
C	-2.66959	0.27395	0.49536
C	-2.14356	-0.56484	-1.70762
C	-3.50577	-0.62934	-2.00574
C	-4.03295	0.20181	0.19953
H	-2.35314	0.63854	1.46802
H	-1.41524	-0.85256	-2.46068
H	-3.82242	-0.97662	-2.98515
H	-4.76257	0.50087	0.94694
H	-5.51481	-0.3075	-1.28401

DAD = 3.0 Å

H in Acceptor Well Total Energy = -1001.18878705

C	-2.4474	-2.9277	0.481
C	-2.5623	-0.1994	-0.1653

C	-1.2798	-2.2262	0.151
C	-3.6606	-2.2562	0.4855
C	-3.7201	-0.8844	0.1623
C	-1.3052	-0.855	-0.1888
H	-4.5703	-2.794	0.736
H	-4.6748	-0.3675	0.1645
H	-2.6064	0.8551	-0.4196
H	2.0275	-4.2683	0.0013
C	2.1559	-3.2245	-0.2669
C	2.4032	-0.5241	-0.9852
C	3.3808	-2.7169	-0.6761
C	1.0505	-2.3695	-0.2122
C	1.1419	-1.0027	-0.5573
C	3.504	-1.3631	-1.0428
H	4.2441	-3.374	-0.7256
H	4.4613	-0.9776	-1.3797
H	2.4991	0.5144	-1.2834
C	0.2275	0.7285	2.4148
H	0.0644	0.2123	0.7191
C	-0.5613	1.9808	2.6592
H	-0.6702	2.121	3.7457
H	-1.5618	1.9273	2.2175
H	-0.0479	2.8589	2.2611
C	1.6957	0.6793	2.7068
H	2.2159	1.537	2.2734
H	2.1406	-0.2484	2.3373
H	1.8356	0.7096	3.7976
O	-0.388	-0.465	2.6263
H	-1.3503	-0.3669	2.7355
C	-0.0474	-0.1414	-0.4431
O	-0.1293	-2.9449	0.1609
C	-0.0922	1.1001	-1.2916
C	-0.1087	3.3297	-3.0066
C	0.5317	2.2967	-0.9133
C	-0.7214	1.0309	-2.5461
C	-0.7252	2.1376	-3.3969
C	0.5203	3.4064	-1.7618
H	1.0298	2.3627	0.0493
H	-1.1968	0.107	-2.8639
H	-1.2125	2.0656	-4.3651
H	1.003	4.3283	-1.4495
H	-0.118	4.1915	-3.6676

H in Donor WellTotal Energy = -1001.18851190

H	-2.3758	-3.9869	0.7106
C	-2.4486	-2.9313	0.4692
C	-2.5635	-0.203	-0.1772

C	-1.2809	-2.2298	0.1391
C	-3.6617	-2.2598	0.4737
C	-3.7212	-0.888	0.1505
C	-1.3064	-0.8586	-0.2006
H	-4.5715	-2.7976	0.7241
H	-4.676	-0.3711	0.1526
H	-2.6076	0.8515	-0.4315
H	2.0263	-4.2719	-0.0106
C	2.1547	-3.2281	-0.2788
C	2.402	-0.5277	-0.9971
C	3.3797	-2.7205	-0.6879
C	1.0493	-2.3731	-0.2241
C	1.1408	-1.0063	-0.5692
C	3.5028	-1.3667	-1.0546
H	4.2429	-3.3776	-0.7375
H	4.4601	-0.9812	-1.3916
H	2.4979	0.5108	-1.2953
C	0.2264	0.7249	2.4029
H	0.1146	0.3711	1.2407
C	-0.5624	1.9772	2.6473
H	-0.6713	2.1174	3.7338
H	-1.563	1.9237	2.2057
H	-0.049	2.8553	2.2493
C	1.6945	0.6757	2.6949
H	2.2147	1.5334	2.2615
H	2.1394	-0.252	2.3255
H	1.8345	0.706	3.7857
O	-0.3891	-0.4686	2.6145
H	-1.3514	-0.3705	2.7237
C	-0.0485	-0.145	-0.455
O	-0.1304	-2.9485	0.149
C	-0.0934	1.0965	-1.3034
C	-0.1099	3.3261	-3.0185
C	0.5305	2.2931	-0.9252
C	-0.7225	1.0273	-2.5579
C	-0.7264	2.134	-3.4088
C	0.5191	3.4028	-1.7737
H	1.0287	2.3591	0.0375
H	-1.1979	0.1034	-2.8757
H	-1.2137	2.062	-4.377
H	1.0019	4.3246	-1.4613
H	-0.1191	4.1879	-3.6795

H at the Midpoint Total Energy = -1001.18569654

H	3.88993	-1.76149	-1.34703
C	2.85097	-1.97759	-1.11952

C	0.14926	-2.46148	-0.53542
C	1.97847	-0.91186	-0.86016
C	2.36268	-3.27489	-1.08258
C	1.0052	-3.52014	-0.78771
C	0.61102	-1.12132	-0.57291
H	3.03169	-4.10574	-1.28668
H	0.63055	-4.53884	-0.76478
H	-0.89704	-2.64753	-0.31355
H	3.43435	2.68169	-1.17257
C	2.37633	2.66752	-0.93106
C	-0.36468	2.55187	-0.34563
C	1.63458	3.83425	-0.81262
C	1.73907	1.4361	-0.74825
C	0.36304	1.34191	-0.44287
C	0.25748	3.7765	-0.52507
H	2.11976	4.79515	-0.95676
H	-0.32009	4.69283	-0.45233
H	-1.42888	2.51147	-0.13959
C	0.26275	-0.29187	2.7174
H	0.00868	-0.13652	1.24725
C	-0.66732	-1.3118	3.3047
H	-0.28694	-1.60494	4.29535
H	-0.73502	-2.21044	2.68275
H	-1.67093	-0.90315	3.44219
C	0.31289	1.10225	3.26257
H	-0.68932	1.52632	3.36173
H	0.92801	1.75032	2.6327
H	0.77115	1.0696	4.2622
O	1.46952	-0.71771	2.25874
H	1.51531	-1.68787	2.19351
C	-0.24546	0.0188	-0.22286
O	2.52054	0.33035	-0.91805
C	-1.72819	-0.11093	-0.4419
C	-4.48365	-0.25295	-0.98949
C	-2.66962	0.23407	0.53734
C	-2.18443	-0.52342	-1.70528
C	-3.55231	-0.58971	-1.97575
C	-4.03846	0.15952	0.26857
H	-2.33229	0.56326	1.51555
H	-1.46981	-0.77979	-2.48258
H	-3.88781	-0.90652	-2.95918
H	-4.75444	0.42416	1.04172
H	-5.5476	-0.31097	-1.20011

DAD = 3.1 Å

H in Acceptor Well Total Energy = -1001.18675766

H	-2.36828	-3.97838	0.74749
C	-2.44352	-2.92673	0.49011
C	-2.56486	-0.2089	-0.19858
C	-1.27878	-2.22962	0.14179
C	-3.65742	-2.25638	0.49109
C	-3.71991	-0.88992	0.14656
C	-1.30745	-0.86373	-0.21897
H	-4.56513	-2.79088	0.75541
H	-4.67512	-0.37377	0.1464
H	-2.61085	0.84194	-0.46739
H	2.03012	-4.27151	-0.00212
C	2.15552	-3.23124	-0.28494
C	2.39542	-0.54003	-1.04116
C	3.37711	-2.72797	-0.70952
C	1.04986	-2.37651	-0.23403
C	1.13761	-1.01409	-0.59799
C	3.49652	-1.37879	-1.09454
H	4.2406	-3.3849	-0.75663
H	4.45123	-0.99703	-1.44298
H	2.48788	0.49447	-1.35393
C	0.23243	0.74353	2.4632
H	0.12247	0.39558	1.32003
C	-0.55683	1.99475	2.7032
H	-0.65748	2.144	3.78959
H	-1.56073	1.9369	2.27
H	-0.04689	2.86992	2.29423
C	1.69902	0.69319	2.75417
H	2.219	1.55039	2.31943
H	2.14303	-0.23521	2.38612
H	1.84	0.72585	3.84521
O	-0.38336	-0.45183	2.66304
H	-1.34845	-0.35586	2.74773
C	-0.05163	-0.15535	-0.48998
O	-0.12675	-2.94682	0.15621
C	-0.09649	1.08615	-1.33842
C	-0.1138	3.31544	-3.05282
C	0.51704	2.28609	-0.95474
C	-0.71712	1.0131	-2.59747
C	-0.72081	2.12013	-3.44806
C	0.5052	3.39582	-1.8031
H	1.00417	2.35314	0.01363
H	-1.18571	0.08669	-2.91815
H	-1.20098	2.04595	-4.41968
H	0.97917	4.32085	-1.48673
H	-0.12322	4.17734	-3.71367

H in Donor WellTotal Energy = -1001.18679738

H	-2.36828	-3.97838	0.74749
C	-2.44352	-2.92673	0.49011
C	-2.56486	-0.2089	-0.19858
C	-1.27878	-2.22962	0.14179
C	-3.65742	-2.25638	0.49109
C	-3.71991	-0.88992	0.14656
C	-1.30745	-0.86373	-0.21897
H	-4.56513	-2.79088	0.75541
H	-4.67512	-0.37377	0.1464
H	-2.61085	0.84194	-0.46739
H	2.03012	-4.27151	-0.00212
C	2.15552	-3.23124	-0.28494
C	2.39542	-0.54003	-1.04116
C	3.37711	-2.72797	-0.70952
C	1.04986	-2.37651	-0.23403
C	1.13761	-1.01409	-0.59799
C	3.49652	-1.37879	-1.09454
H	4.2406	-3.3849	-0.75663
H	4.45123	-0.99703	-1.44298
H	2.48788	0.49447	-1.35393
C	0.23243	0.74353	2.4632
H	0.05833	0.1926	0.65318
C	-0.55683	1.99475	2.7032
H	-0.65748	2.144	3.78959
H	-1.56073	1.9369	2.27
H	-0.04689	2.86992	2.29423
C	1.69902	0.69319	2.75417
H	2.219	1.55039	2.31943
H	2.14303	-0.23521	2.38612
H	1.84	0.72585	3.84521
O	-0.38336	-0.45183	2.66304
H	-1.34845	-0.35586	2.74773
C	-0.05163	-0.15535	-0.48998
O	-0.12675	-2.94682	0.15621
C	-0.09649	1.08615	-1.33842
C	-0.1138	3.31544	-3.05282
C	0.51704	2.28609	-0.95474
C	-0.71712	1.0131	-2.59747
C	-0.72081	2.12013	-3.44806
C	0.5052	3.39582	-1.8031
H	1.00417	2.35314	0.01363
H	-1.18571	0.08669	-2.91815
H	-1.20098	2.04595	-4.41968
H	0.97917	4.32085	-1.48673
H	-0.12322	4.17734	-3.71367

H at the Midpoint Total Energy = -1001.18101627

H	3.88143	-1.70326	-1.4313
C	2.84509	-1.93086	-1.20307
C	0.14922	-2.44434	-0.61638
C	1.96674	-0.87648	-0.91898
C	2.36559	-3.23194	-1.18988
C	1.01112	-3.49183	-0.89377
C	0.60208	-1.10083	-0.62917
H	3.03903	-4.0541	-1.41354
H	0.64329	-4.51337	-0.88924
H	-0.89442	-2.64157	-0.3915
H	3.39455	2.73405	-1.17251
C	2.33842	2.70703	-0.92405
C	-0.39805	2.55945	-0.32238
C	1.58851	3.86564	-0.77875
C	1.71171	1.46768	-0.76011
C	0.33831	1.3572	-0.44715
C	0.21391	3.79181	-0.48242
H	2.06519	4.83278	-0.90841
H	-0.36995	4.70224	-0.38836
H	-1.46046	2.50665	-0.11011
C	0.3343	-0.36114	2.76638
H	0.03844	-0.16724	1.25728
C	-0.57748	-1.40045	3.34478
H	-0.18293	-1.70754	4.32594
H	-0.64436	-2.28876	2.70817
H	-1.5829	-1.00316	3.50141
C	0.38756	1.01909	3.34101
H	-0.61525	1.43379	3.46975
H	0.98627	1.68496	2.71436
H	0.86511	0.96702	4.33124
O	1.52993	-0.76569	2.26157
H	1.57113	-1.73194	2.14996
C	-0.25741	0.02665	-0.25182
O	2.50003	0.37096	-0.95432
C	-1.74355	-0.10844	-0.44246
C	-4.5084	-0.25791	-0.93479
C	-2.66564	0.19552	0.5679
C	-2.22337	-0.4849	-1.70886
C	-3.59642	-0.55451	-1.95153
C	-4.03929	0.11716	0.32644
H	-2.30697	0.4925	1.54907
H	-1.52354	-0.71057	-2.50883
H	-3.95102	-0.84286	-2.93705
H	-4.74043	0.34901	1.12334
H	-5.57619	-0.31866	-1.12407

DAD = 3.2 Å

H in Acceptor Well Total Energy = -1001.18473370

H	-2.35256	-3.95723	0.82512
C	-2.43279	-2.91233	0.54292
C	-2.56719	-0.21238	-0.21223
C	-1.27185	-2.21864	0.17625
C	-3.65	-2.24781	0.52799
C	-3.71893	-0.89076	0.14935
C	-1.30682	-0.86146	-0.21643
H	-4.55515	-2.77991	0.80573
H	-4.67668	-0.37945	0.13625
H	-2.61789	0.83153	-0.50588
H	2.04321	-4.25403	0.05643
C	2.16297	-3.21984	-0.25011
C	2.38874	-0.54484	-1.06787
C	3.3791	-2.72273	-0.69735
C	1.05568	-2.36709	-0.20834
C	1.13654	-1.01234	-0.60234
C	3.49127	-1.38206	-1.11326
H	4.24389	-3.37834	-0.7384
H	4.44161	-1.00594	-1.47928
H	2.47488	0.48258	-1.40461
C	0.23938	0.77073	2.54404
H	0.05611	0.1908	0.63876
C	-0.54865	2.0228	2.77581
H	-0.62859	2.19199	3.86133
H	-1.56054	1.95549	2.36317
H	-0.0476	2.89134	2.34169
C	1.70527	0.7215	2.83274
H	2.22547	1.57262	2.38662
H	2.1472	-0.21233	2.47696
H	1.84767	0.76941	3.92326
O	-0.37663	-0.42642	2.73216
H	-1.34323	-0.33145	2.7979
C	-0.05385	-0.15715	-0.5044
O	-0.11598	-2.93014	0.20603
C	-0.09984	1.0769	-1.36359
C	-0.1199	3.29145	-3.09513
C	0.49964	2.28503	-0.98253
C	-0.70855	0.98768	-2.62735
C	-0.71321	2.08792	-3.48676
C	0.48621	3.38773	-1.84
H	0.97405	2.36256	-0.00843
H	-1.16679	0.05475	-2.94436
H	-1.18368	2.00223	-4.46223

H	0.9484	4.31977	-1.52654
H	-0.1304	4.14787	-3.76308

H in Donor WellTotal Energy = -1001.18461956

C	-3.65163	-2.25297	0.51106
C	-3.72056	-0.89591	0.13241
C	-1.30845	-0.86662	-0.23337
H	-4.55678	-2.78506	0.78879
H	-4.67831	-0.3846	0.11931
H	-2.61952	0.82637	-0.52281
H	2.04158	-4.25918	0.0395
C	2.16134	-3.225	-0.26705
C	2.38711	-0.54999	-1.08481
C	3.37747	-2.72788	-0.71429
C	1.05405	-2.37224	-0.22527
C	1.13491	-1.0175	-0.61928
C	3.48964	-1.38722	-1.1302
H	4.24226	-3.3835	-0.75533
H	4.43998	-1.0111	-1.49622
H	2.47325	0.47743	-1.42155
C	0.23775	0.76557	2.52711
H	0.12779	0.41762	1.38394
C	-0.55027	2.01765	2.75888
H	-0.63022	2.18683	3.84439
H	-1.56217	1.95034	2.34623
H	-0.04923	2.88618	2.32475
C	1.70364	0.71634	2.8158
H	2.22384	1.56747	2.36969
H	2.14557	-0.21748	2.46003
H	1.84604	0.76425	3.90633
O	-0.37826	-0.43158	2.71522
H	-1.34486	-0.3366	2.78097
C	-0.05547	-0.16231	-0.52134
O	-0.11761	-2.93529	0.18909
C	-0.10147	1.07174	-1.38053
C	-0.12153	3.28629	-3.11206
C	0.49801	2.27988	-0.99947
C	-0.71017	0.98253	-2.64429
C	-0.71484	2.08277	-3.5037
C	0.48458	3.38258	-1.85694
H	0.97242	2.3574	-0.02536
H	-1.16842	0.0496	-2.9613
H	-1.18531	1.99707	-4.47917
H	0.94677	4.31461	-1.54347
H	-0.13203	4.14272	-3.78002

H at the Midpoint Total Energy = -1001.17563215

H	3.86585	-1.63376	-1.52431
C	2.83448	-1.87675	-1.28948
C	0.14973	-2.42984	-0.68598
C	1.94845	-0.83772	-0.97516
C	2.36805	-3.18279	-1.29876
C	1.01922	-3.46228	-0.99501
C	0.58931	-1.08207	-0.67453
H	3.04723	-3.99327	-1.54656
H	0.66144	-4.48732	-1.00892
H	-0.88927	-2.64219	-0.45373
H	3.33073	2.79397	-1.19179
C	2.27803	2.74999	-0.93154
C	-0.44984	2.55974	-0.30078
C	1.51459	3.89681	-0.76395
C	1.66903	1.501	-0.77606
C	0.30077	1.36888	-0.44815
C	0.14445	3.80159	-0.45319
H	1.97705	4.8716	-0.88759
H	-0.44994	4.70321	-0.34201
H	-1.50901	2.4901	-0.07777
C	0.44979	-0.41497	2.81982
H	0.08775	-0.19271	1.27725
C	-0.43413	-1.47229	3.40562
H	-0.02136	-1.77482	4.38105
H	-0.4937	-2.36001	2.76754
H	-1.44423	-1.09268	3.57726
C	0.50512	0.95557	3.41408
H	-0.49788	1.35932	3.57227
H	1.08485	1.63594	2.78566
H	1.00415	0.89119	4.39318
O	1.62722	-0.79431	2.25611
H	1.66705	-1.75592	2.10987
C	-0.27428	0.02954	-0.26532
O	2.46826	0.41636	-0.99117
C	-1.76348	-0.1181	-0.41927
C	-4.53778	-0.28957	-0.83966
C	-2.66017	0.14307	0.62567
C	-2.27257	-0.46365	-1.68299
C	-3.65096	-0.54389	-1.88978
C	-4.03888	0.05355	0.41945
H	-2.27575	0.41265	1.60521
H	-1.59211	-0.65683	-2.50791
H	-4.02943	-0.80775	-2.87332
H	-4.72074	0.25133	1.24196
H	-5.60957	-0.35882	-1.00152

DAD = 3.3 Å

H in Acceptor Well Total Energy = -1001.18272089

H	-2.34337	-3.96177	0.83206
C	-2.42767	-2.9204	0.53818
C	-2.57291	-0.22967	-0.2488
C	-1.26969	-2.22588	0.16498
C	-3.64792	-2.26164	0.51281
C	-3.72217	-0.90969	0.11759
C	-1.30957	-0.87272	-0.24181
H	-4.55124	-2.79463	0.79467
H	-4.68237	-0.4033	0.09558
H	-2.62777	0.81057	-0.55429
H	2.05337	-4.25129	0.06003
C	2.16826	-3.21989	-0.2575
C	2.38257	-0.55179	-1.10259
C	3.38138	-2.72257	-0.71295
C	1.05811	-2.37081	-0.22177
C	1.13308	-1.01948	-0.6295
C	3.48778	-1.38559	-1.14247
H	4.24854	-3.37534	-0.74969
H	4.43599	-1.0099	-1.51445
H	2.4639	0.47271	-1.44912
C	0.24359	0.78682	2.60724
H	0.04932	0.1721	0.58765
C	-0.54562	2.03825	2.83156
H	-0.62198	2.21515	3.91625
H	-1.55859	1.96739	2.42304
H	-0.04622	2.90393	2.39005
C	1.7077	0.7379	2.89711
H	2.22911	1.58485	2.44443
H	2.14879	-0.19972	2.55121
H	1.8484	0.79675	3.98775
O	-0.37261	-0.41202	2.78362
H	-1.3407	-0.3189	2.82456
C	-0.05881	-0.17006	-0.53647
O	-0.11015	-2.93182	0.20411
C	-0.10366	1.07145	-1.38491
C	-0.1194	3.29913	-3.09919
C	0.48985	2.27783	-0.99043
C	-0.70482	0.99044	-2.65302
C	-0.70715	2.09744	-3.50385
C	0.47847	3.38695	-1.83948
H	0.9566	2.34767	-0.01209
H	-1.15866	0.05883	-2.98013
H	-1.17144	2.01826	-4.48277
H	0.9358	4.31787	-1.51589

H	-0.12798	4.1608	-3.76038

H in Donor WellTotal Energy = -1001.18279958

H	-2.3452	-3.96757	0.81301
C	-2.4295	-2.9262	0.51912
C	-2.57475	-0.23547	-0.26785
C	-1.27152	-2.23168	0.14593
C	-3.64975	-2.26744	0.49375
C	-3.724	-0.91549	0.09854
C	-1.3114	-0.87852	-0.26086
H	-4.55307	-2.80043	0.77561
H	-4.6842	-0.4091	0.07653
H	-2.6296	0.80477	-0.57334
H	2.05154	-4.25709	0.04098
C	2.16643	-3.22568	-0.27655
C	2.38074	-0.55759	-1.12164
C	3.37955	-2.72837	-0.73201
C	1.05627	-2.37661	-0.24082
C	1.13125	-1.02528	-0.64855
C	3.48595	-1.39139	-1.16152
H	4.24671	-3.38114	-0.76874
H	4.43416	-1.0157	-1.53351
H	2.46207	0.46691	-1.46818
C	0.24175	0.78102	2.58819
H	0.13363	0.43886	1.46407
C	-0.54745	2.03245	2.81251
H	-0.62381	2.20935	3.8972
H	-1.56042	1.96159	2.40399
H	-0.04805	2.89813	2.371
C	1.70587	0.7321	2.87806
H	2.22727	1.57905	2.42538
H	2.14696	-0.20552	2.53216
H	1.84656	0.79095	3.96869
O	-0.37444	-0.41782	2.76457
H	-1.34254	-0.3247	2.80551
C	-0.06064	-0.17586	-0.55552
O	-0.11198	-2.93762	0.18506
C	-0.10549	1.06565	-1.40396
C	-0.12124	3.29333	-3.11825
C	0.48802	2.27204	-1.00948
C	-0.70665	0.98464	-2.67207
C	-0.70898	2.09164	-3.52291
C	0.47664	3.38115	-1.85853
H	0.95476	2.34187	-0.03114
H	-1.16049	0.05303	-2.99918
H	-1.17327	2.01246	-4.50182
H	0.93397	4.31207	-1.53494

H	-0.12981	4.155	-3.77943

H at the Midpoint Total Energy = -1001.17015870

H	3.86224	-1.59672	-1.57275
C	2.83135	-1.8465	-1.34296
C	0.14683	-2.41718	-0.75292
C	1.94176	-0.81567	-1.01346
C	2.36838	-3.15349	-1.37513
C	1.01977	-3.44149	-1.07884
C	0.58301	-1.06882	-0.71709
H	3.05006	-3.9578	-1.63571
H	0.66461	-4.46701	-1.11161
H	-0.89177	-2.63633	-0.52551
H	3.30982	2.82521	-1.18213
C	2.25707	2.773	-0.92366
C	-0.47092	2.56278	-0.29698
C	1.48794	3.91409	-0.74257
C	1.65352	1.51963	-0.78426
C	0.28539	1.37722	-0.45886
C	0.11792	3.80891	-0.43386
H	1.94592	4.8925	-0.85384
H	-0.48041	4.70654	-0.31193
H	-1.5297	2.4852	-0.07504
C	0.49865	-0.45845	2.8751
H	0.10861	-0.21182	1.29094
C	-0.37946	-1.52479	3.45049
H	0.03667	-1.83551	4.42206
H	-0.43769	-2.40621	2.80417
H	-1.39009	-1.14983	3.62873
C	0.55655	0.90324	3.48542
H	-0.4459	1.30537	3.65124
H	1.13636	1.5908	2.86542
H	1.05652	0.82492	4.4635
O	1.66681	-0.82533	2.28448
H	1.69683	-1.78151	2.10458
C	-0.28144	0.03482	-0.2932
O	2.45754	0.44066	-1.00856
C	-1.77259	-0.11793	-0.42102
C	-4.55315	-0.2946	-0.7936
C	-2.65047	0.12053	0.64467
C	-2.30334	-0.44395	-1.68121
C	-3.68505	-0.52666	-1.86401
C	-4.03223	0.02835	0.46194
H	-2.24752	0.37331	1.62119
H	-1.63742	-0.61966	-2.52178
H	-4.08057	-0.77498	-2.84483

H	-4.6997	0.2082	1.30017
H	-5.62747	-0.36567	-0.93679

DAD = 3.5 Å

H in Acceptor Well Total Energy = -1001.17911154

H	-2.3589	-4.04161	0.62829
C	-2.44283	-2.99143	0.36755
C	-2.58653	-0.27614	-0.33132
C	-1.2828	-2.28053	0.03538
C	-3.66525	-2.33665	0.34383
C	-3.73814	-0.97238	-0.00642
C	-1.32051	-0.91436	-0.32579
H	-4.57096	-2.88204	0.59241
H	-4.69993	-0.46888	-0.02667
H	-2.6413	0.77372	-0.60133
H	2.05418	-4.28535	-0.06982
C	2.16823	-3.24471	-0.3559
C	2.38202	-0.55136	-1.11959
C	3.38672	-2.72672	-0.77167
C	1.05197	-2.40377	-0.31835
C	1.12588	-1.04034	-0.68597
C	3.49296	-1.37676	-1.15994
H	4.25896	-3.37265	-0.80936
H	4.44633	-0.98499	-1.50088
H	2.46376	0.48379	-1.43243
C	0.24948	0.80789	2.73938
H	0.03598	0.13227	0.51973
C	-0.54102	2.05822	2.94939
H	-0.607	2.25305	4.03215
H	-1.55698	1.97791	2.55096
H	-0.04692	2.91759	2.48978
C	1.71236	0.75853	3.02295
H	2.23295	1.6027	2.56427
H	2.15011	-0.18202	2.6819
H	1.85586	0.82607	4.11332
O	-0.36692	-0.39407	2.89223
H	-1.33536	-0.29933	2.91766
C	-0.07123	-0.20698	-0.59486
O	-0.11959	-2.98177	0.07198
C	-0.1092	1.07724	-1.37749
C	-0.09785	3.38569	-2.98375
C	0.50052	2.25644	-0.92725
C	-0.7125	1.06616	-2.64714
C	-0.70175	2.2128	-3.44421
C	0.50274	3.40445	-1.72212

H	0.96684	2.27109	0.05347
H	-1.1775	0.1573	-3.01955
H	-1.16813	2.18623	-4.42498
H	0.9726	4.31281	-1.35503
H	-0.09591	4.27841	-3.60243

H in Donor WellTotal Energy = -1001.17903071

H	-2.36105	-4.04844	0.60585
C	-2.44499	-2.99826	0.34511
C	-2.58869	-0.28297	-0.35376
C	-1.28496	-2.28736	0.01294
C	-3.66741	-2.34348	0.32139
C	-3.7403	-0.97921	-0.02886
C	-1.32267	-0.92119	-0.34823
H	-4.57312	-2.88887	0.56997
H	-4.70209	-0.47571	-0.04911
H	-2.64346	0.76689	-0.62377
H	2.05202	-4.29218	-0.09226
C	2.16607	-3.25154	-0.37834
C	2.37986	-0.55819	-1.14203
C	3.38456	-2.73355	-0.79411
C	1.04981	-2.4106	-0.34079
C	1.12372	-1.04717	-0.70841
C	3.49081	-1.38359	-1.18238
H	4.2568	-3.37948	-0.8318
H	4.44417	-0.99182	-1.52332
H	2.4616	0.47696	-1.45487
C	0.24733	0.80106	2.71694
H	0.14011	0.4618	1.60235
C	-0.54318	2.05139	2.92695
H	-0.60916	2.24622	4.00971
H	-1.55914	1.97108	2.52852
H	-0.04908	2.91076	2.46734
C	1.7102	0.7517	3.00051
H	2.2308	1.59587	2.54183
H	2.14795	-0.18885	2.65946
H	1.8537	0.81924	4.09088
O	-0.36908	-0.4009	2.86979
H	-1.33752	-0.30616	2.89522
C	-0.07339	-0.21381	-0.6173
O	-0.12175	-2.9886	0.04954
C	-0.11136	1.07041	-1.39993
C	-0.1	3.37886	-3.00619
C	0.49836	2.24961	-0.94969
C	-0.71466	1.05933	-2.66958
C	-0.70391	2.20597	-3.46665
C	0.50058	3.39762	-1.74456

H	0.96468	2.26426	0.03103
H	-1.17966	0.15047	-3.04199
H	-1.17029	2.1794	-4.44742
H	0.97044	4.30598	-1.37747
H	-0.09807	4.27158	-3.62487

H at the Midpoint Total Energy = -1001.15940742

H	3.89594	-1.67817	-1.49579
C	2.85372	-1.90694	-1.29743
C	0.14154	-2.42316	-0.78798
C	1.97456	-0.85867	-0.99815
C	2.36593	-3.20452	-1.34185
C	1.00369	-3.46472	-1.08528
C	0.60269	-1.08325	-0.74159
H	3.03888	-4.02281	-1.58079
H	0.62952	-4.48317	-1.12657
H	-0.90708	-2.62203	-0.59062
H	3.42121	2.75504	-1.11726
C	2.35918	2.7238	-0.89612
C	-0.39327	2.56863	-0.36414
C	1.60786	3.87972	-0.73717
C	1.72546	1.48284	-0.78187
C	0.34367	1.36769	-0.50452
C	0.22586	3.80207	-0.47554
H	2.08934	4.84884	-0.82897
H	-0.35715	4.71186	-0.37053
H	-1.45991	2.51211	-0.17662
C	0.34251	-0.44914	3.0474
H	0.04521	-0.20442	1.34029
C	-0.60272	-1.48339	3.56625
H	-0.27591	-1.78148	4.57572
H	-0.6276	-2.37627	2.93419
H	-1.61537	-1.08227	3.65313
C	0.39217	0.92032	3.63474
H	-0.60882	1.34968	3.72252
H	1.03295	1.58037	3.04625
H	0.81755	0.84674	4.6485
O	1.52906	-0.84844	2.51762
H	1.53841	-1.80559	2.34079
C	-0.25209	0.0403	-0.36681
O	2.51437	0.38804	-0.97688
C	-1.74358	-0.09217	-0.51219
C	-4.52225	-0.21693	-0.92754
C	-2.63432	0.19455	0.53152
C	-2.26195	-0.44015	-1.77167
C	-3.64224	-0.49733	-1.97603
C	-4.0141	0.12848	0.32755

H	-2.23933	0.46252	1.50706
H	-1.5874	-0.65172	-2.59699
H	-4.02668	-0.76313	-2.95669
H	-4.69104	0.34581	1.14923
H	-5.59547	-0.268	-1.0866

Table S4. The atom coordinates and absolute energies of the TRS at different DADs for the reaction of $PhTXn^{+}$ (for Table 1 data in the paper)

DAD = 2.8 Å

H in Acceptor Well Total Energy = -1324.15488274

H	-2.83564	-3.86189	0.69361
C	-2.75194	-2.80532	0.4531
C	-2.5353	-0.10042	-0.18241
C	-1.47956	-2.25175	0.19763
C	-3.88727	-2.01453	0.39621
C	-3.77889	-0.64725	0.07845
C	-1.34703	-0.88063	-0.14013
H	-4.86032	-2.45526	0.59286
H	-4.66762	-0.02548	0.02871
H	-2.45596	0.94969	-0.44165
H	2.4747	-4.176	0.01124
C	2.45588	-3.11912	-0.24151
C	2.39051	-0.42059	-0.9278
C	3.61492	-2.4836	-0.65749
C	1.24258	-2.40794	-0.15739
C	1.18651	-1.03074	-0.49018
C	3.57967	-1.12424	-1.01094
H	4.54312	-3.04391	-0.72148
H	4.48041	-0.62547	-1.3555
H	2.37372	0.62475	-1.21296
C	0.2121	0.60014	2.31515
H	0.07465	0.16519	0.88618
C	-0.5402	1.87276	2.59128
H	-0.69433	1.95148	3.678
H	-1.52187	1.88327	2.10575
H	0.01946	2.75403	2.27229
C	1.68113	0.5172	2.61005
H	2.22349	1.35311	2.16122
H	2.10344	-0.42696	2.25567
H	1.82029	0.56158	3.69983
O	-0.43605	-0.56544	2.58301
H	-1.39132	-0.4338	2.7119
C	-0.04448	-0.21176	-0.35225
S	-0.14364	-3.36843	0.31502

C	-0.08839	1.02146	-1.22724
C	-0.12043	3.20387	-3.00748
C	0.38376	2.27659	-0.82782
C	-0.56874	0.86921	-2.54081
C	-0.58132	1.95055	-3.42202
C	0.36226	3.3636	-1.70765
H	0.77989	2.41469	0.17249
H	-0.92793	-0.10045	-2.87491
H	-0.95314	1.81178	-4.43336
H	0.72664	4.33151	-1.37463
H	-0.13609	4.04652	-3.69257

H in Donor WellTotal Energy = -1324.15503972

H	-2.83564	-3.86189	0.69361
C	-2.75194	-2.80532	0.4531
C	-2.5353	-0.10042	-0.18241
C	-1.47956	-2.25175	0.19763
C	-3.88727	-2.01453	0.39621
C	-3.77889	-0.64725	0.07845
C	-1.34703	-0.88063	-0.14013
H	-4.86032	-2.45526	0.59286
H	-4.66762	-0.02548	0.02871
H	-2.45596	0.94969	-0.44165
H	2.4747	-4.176	0.01124
C	2.45588	-3.11912	-0.24151
C	2.39051	-0.42059	-0.9278
C	3.61492	-2.4836	-0.65749
C	1.24258	-2.40794	-0.15739
C	1.18651	-1.03074	-0.49018
C	3.57967	-1.12424	-1.01094
H	4.54312	-3.04391	-0.72148
H	4.48041	-0.62547	-1.3555
H	2.37372	0.62475	-1.21296
C	0.2121	0.60014	2.31515
H	0.09297	0.22319	1.07671
C	-0.5402	1.87276	2.59128
H	-0.69433	1.95148	3.678
H	-1.52187	1.88327	2.10575
H	0.01946	2.75403	2.27229
C	1.68113	0.5172	2.61005
H	2.22349	1.35311	2.16122
H	2.10344	-0.42696	2.25567
H	1.82029	0.56158	3.69983
O	-0.43605	-0.56544	2.58301
H	-1.39132	-0.4338	2.7119
C	-0.04448	-0.21176	-0.35225
S	-0.14364	-3.36843	0.31502

C	-0.08839	1.02146	-1.22724
C	-0.12043	3.20387	-3.00748
C	0.38376	2.27659	-0.82782
C	-0.56874	0.86921	-2.54081
C	-0.58132	1.95055	-3.42202
C	0.36226	3.3636	-1.70765
H	0.77989	2.41469	0.17249
H	-0.92793	-0.10045	-2.87491
H	-0.95314	1.81178	-4.43336
H	0.72664	4.33151	-1.37463
H	-0.13609	4.04652	-3.69257

H at the midpoint Total Energy = -1324.15492613

H	3.61455	-2.40949	-1.19129
C	2.55339	-2.42939	-0.95741
C	-0.17188	-2.47538	-0.37593
C	1.87007	-1.2151	-0.73561
C	1.88198	-3.63815	-0.88194
C	0.50596	-3.66297	-0.5851
C	0.48063	-1.21398	-0.45085
H	2.42079	-4.56475	-1.05756
H	-0.02431	-4.60883	-0.52954
H	-1.23496	-2.49623	-0.16221
H	3.29534	2.94083	-1.00122
C	2.23469	2.82177	-0.79611
C	-0.48991	2.50623	-0.31205
C	1.41563	3.93575	-0.70405
C	1.69985	1.52764	-0.64088
C	0.31812	1.34194	-0.38219
C	0.03997	3.77556	-0.46754
H	1.83961	4.92781	-0.82917
H	-0.61004	4.64351	-0.41303
H	-1.55408	2.39498	-0.14032
C	0.09921	-0.1987	2.6274
H	-0.09542	-0.0946	1.24491
C	-0.88764	-1.13686	3.26595
H	-0.48634	-1.44385	4.24352
H	-1.04647	-2.03799	2.66406
H	-1.85198	-0.65619	3.44088
C	0.21353	1.21614	3.11431
H	-0.7642	1.70296	3.15139
H	0.88991	1.7987	2.48303
H	0.62991	1.20136	4.13183
O	1.30359	-0.72333	2.27435
H	1.29581	-1.69617	2.27655
C	-0.29005	0.00951	-0.13758
S	2.84965	0.22415	-0.85582

C	-1.77368	-0.07333	-0.42102
C	-4.50075	-0.14401	-1.12197
C	-2.76408	0.17761	0.53499
C	-2.16806	-0.3502	-1.74283
C	-3.5191	-0.38209	-2.08879
C	-4.11912	0.13604	0.19104
H	-2.48554	0.41545	1.55601
H	-1.41413	-0.53517	-2.50327
H	-3.80316	-0.59447	-3.11568
H	-4.87223	0.32648	0.9507
H	-5.55253	-0.17484	-1.39115

DAD = 2.9 Å

H in Acceptor Well Total Energy = -1324.15297447

H	-2.82954	-3.85415	0.73148
C	-2.74765	-2.80103	0.4757
C	-2.53562	-0.10489	-0.19943
C	-1.47735	-2.25129	0.20202
C	-3.88325	-2.01076	0.41664
C	-3.77692	-0.64796	0.07899
C	-1.34724	-0.88489	-0.15613
H	-4.85488	-2.44826	0.62703
H	-4.66598	-0.02673	0.02801
H	-2.45758	0.94201	-0.47167
H	2.47946	-4.17489	0.0203
C	2.45823	-3.12079	-0.24365
C	2.38737	-0.429	-0.95766
C	3.61563	-2.48714	-0.66724
C	1.24386	-2.41098	-0.16576
C	1.18459	-1.03745	-0.51393
C	3.57773	-1.1312	-1.0339
H	4.54487	-3.04626	-0.72639
H	4.47755	-0.63431	-1.38354
H	2.36766	0.61355	-1.2528
C	0.21865	0.61877	2.37521
H	0.06654	0.13743	0.79382
C	-0.53337	1.89023	2.6472
H	-0.68132	1.97889	3.73435
H	-1.51746	1.89667	2.16669
H	0.02534	2.76836	2.3172
C	1.68711	0.53183	2.66408
H	2.22927	1.36567	2.21112
H	2.10457	-0.41428	2.30936
H	1.83296	0.57828	3.75338
O	-0.4304	-0.55141	2.6198

H	-1.3873	-0.4222	2.73981
C	-0.04709	-0.22212	-0.38745
S	-0.14022	-3.36668	0.32182
C	-0.091	1.0111	-1.26245
C	-0.12979	3.19679	-3.03637
C	0.35974	2.27091	-0.85285
C	-0.55568	0.85558	-2.58077
C	-0.57123	1.93919	-3.45933
C	0.33548	3.35957	-1.73039
H	0.73956	2.40926	0.15396
H	-0.90022	-0.11747	-2.92068
H	-0.93022	1.79894	-4.47509
H	0.6835	4.33132	-1.39105
H	-0.14765	4.04085	-3.7197

H in Donor WellTotal Energy = -1324.15312463

H	-2.82954	-3.85415	0.73148
C	-2.74765	-2.80103	0.4757
C	-2.53562	-0.10489	-0.19943
C	-1.47735	-2.25129	0.20202
C	-3.88325	-2.01076	0.41664
C	-3.77692	-0.64796	0.07899
C	-1.34724	-0.88489	-0.15613
H	-4.85488	-2.44826	0.62703
H	-4.66598	-0.02673	0.02801
H	-2.45758	0.94201	-0.47167
H	2.47946	-4.17489	0.0203
C	2.45823	-3.12079	-0.24365
C	2.38737	-0.429	-0.95766
C	3.61563	-2.48714	-0.66724
C	1.24386	-2.41098	-0.16576
C	1.18459	-1.03745	-0.51393
C	3.57773	-1.1312	-1.0339
H	4.54487	-3.04626	-0.72639
H	4.47755	-0.63431	-1.38354
H	2.36766	0.61355	-1.2528
C	0.21865	0.61877	2.37521
H	0.10502	0.25922	1.19393
C	-0.53337	1.89023	2.6472
H	-0.68132	1.97889	3.73435
H	-1.51746	1.89667	2.16669
H	0.02534	2.76836	2.3172
C	1.68711	0.53183	2.66408
H	2.22927	1.36567	2.21112
H	2.10457	-0.41428	2.30936

H	1.83296	0.57828	3.75338
O	-0.4304	-0.55141	2.6198
H	-1.3873	-0.4222	2.73981
C	-0.04709	-0.22212	-0.38745
S	-0.14022	-3.36668	0.32182
C	-0.091	1.0111	-1.26245
C	-0.12979	3.19679	-3.03637
C	0.35974	2.27091	-0.85285
C	-0.55568	0.85558	-2.58077
C	-0.57123	1.93919	-3.45933
C	0.33548	3.35957	-1.73039
H	0.73956	2.40926	0.15396
H	-0.90022	-0.11747	-2.92068
H	-0.93022	1.79894	-4.47509
H	0.6835	4.33132	-1.39105
H	-0.14765	4.04085	-3.7197

H at the Midpoint Total Energy = -1324.15193480

H	3.59796	-2.40342	-1.24259
C	2.5371	-2.42286	-1.00725
C	-0.18793	-2.46731	-0.42229
C	1.85626	-1.20878	-0.77654
C	1.86324	-3.6307	-0.93921
C	0.48748	-3.65453	-0.6405
C	0.46697	-1.20673	-0.48998
H	2.39971	-4.55727	-1.12195
H	-0.04444	-4.59979	-0.59036
H	-1.25026	-2.4873	-0.20491
H	3.28971	2.94846	-1.00505
C	2.22986	2.82899	-0.79604
C	-0.49333	2.51343	-0.30083
C	1.41382	3.94345	-0.68388
C	1.69261	1.53428	-0.65568
C	0.3114	1.34823	-0.39304
C	0.03911	3.78336	-0.44103
H	1.83944	4.93618	-0.79765
H	-0.60809	4.65222	-0.37003
H	-1.55664	2.40153	-0.12404
C	0.15044	-0.23906	2.68557
H	-0.07384	-0.1117	1.25869
C	-0.82936	-1.18213	3.32332
H	-0.42229	-1.49839	4.29591
H	-0.99431	-2.07734	2.71443
H	-1.79144	-0.70032	3.50886
C	0.27738	1.16973	3.18214
H	-0.69826	1.65915	3.23685
H	0.94696	1.75449	2.54578

H	0.70759	1.14674	4.19426
O	1.34149	-0.75883	2.28351
H	1.32946	-1.73157	2.26372
C	-0.29811	0.01567	-0.16819
S	2.83754	0.23015	-0.89052
C	-1.78633	-0.05968	-0.42877
C	-4.52428	-0.12218	-1.08087
C	-2.75912	0.15791	0.55327
C	-2.20265	-0.30146	-1.75025
C	-3.55986	-0.32896	-2.07205
C	-4.11994	0.12105	0.23287
H	-2.46005	0.36445	1.5755
H	-1.46184	-0.46253	-2.52892
H	-3.86227	-0.51353	-3.09908
H	-4.86001	0.28578	1.01115
H	-5.58071	-0.14939	-1.33172

DAD = 3.0 Å

H in Acceptor Well Total Energy = -1324.15137378

H	-2.82147	-3.83767	0.79047
C	-2.74202	-2.7895	0.51441
C	-2.53589	-0.1061	-0.21307
C	-1.47384	-2.24387	0.22325
C	-3.8786	-2.00132	0.44628
C	-3.77495	-0.64495	0.08256
C	-1.34677	-0.88434	-0.16197
H	-4.84881	-2.43525	0.67018
H	-4.66478	-0.02535	0.02528
H	-2.4598	0.936	-0.50347
H	2.48436	-4.16825	0.04851
C	2.46078	-3.11807	-0.23048
C	2.38418	-0.43629	-0.9821
C	3.61572	-2.48918	-0.66785
C	1.24616	-2.40833	-0.15739
C	1.18348	-1.04019	-0.52651
C	3.57499	-1.13819	-1.05242
H	4.54536	-3.04799	-0.72301
H	4.47317	-0.64513	-1.41159
H	2.362	0.60219	-1.29112
C	0.22606	0.64225	2.44472
H	0.06204	0.12321	0.73949
C	-0.52442	1.91553	2.70517
H	-0.66014	2.02395	3.7924
H	-1.51356	1.91377	2.23524
H	0.03133	2.78734	2.35321
C	1.69446	0.55423	2.72638

H	2.23556	1.38196	2.261
H	2.10645	-0.39679	2.37887
H	1.84838	0.6126	3.81438
O	-0.42336	-0.53011	2.67764
H	-1.38259	-0.40243	2.78168
C	-0.04884	-0.22764	-0.4132
S	-0.13429	-3.3556	0.35599
C	-0.0939	0.99789	-1.29887
C	-0.14023	3.172	-3.08476
C	0.33863	2.26498	-0.89097
C	-0.54675	0.82908	-2.61883
C	-0.5655	1.90762	-3.50388
C	0.31115	3.3479	-1.77553
H	0.70464	2.41143	0.12019
H	-0.87936	-0.14934	-2.9553
H	-0.91461	1.75797	-4.52174
H	0.64522	4.32555	-1.43922
H	-0.16055	4.01153	-3.77354

H in Donor WellTotal Energy = -1324.15174851

H	-2.82147	-3.83767	0.79047
C	-2.74202	-2.7895	0.51441
C	-2.53589	-0.1061	-0.21307
C	-1.47384	-2.24387	0.22325
C	-3.8786	-2.00132	0.44628
C	-3.77495	-0.64495	0.08256
C	-1.34677	-0.88434	-0.16197
H	-4.84881	-2.43525	0.67018
H	-4.66478	-0.02535	0.02528
H	-2.4598	0.936	-0.50347
H	2.48436	-4.16825	0.04851
C	2.46078	-3.11807	-0.23048
C	2.38418	-0.43629	-0.9821
C	3.61572	-2.48918	-0.66785
C	1.24616	-2.40833	-0.15739
C	1.18348	-1.04019	-0.52651
C	3.57499	-1.13819	-1.05242
H	4.54536	-3.04799	-0.72301
H	4.47317	-0.64513	-1.41159
H	2.362	0.60219	-1.29112
C	0.22606	0.64225	2.44472
H	0.11518	0.29139	1.29202
C	-0.52442	1.91553	2.70517
H	-0.66014	2.02395	3.7924
H	-1.51356	1.91377	2.23524

H	0.03133	2.78734	2.35321
C	1.69446	0.55423	2.72638
H	2.23556	1.38196	2.261
H	2.10645	-0.39679	2.37887
H	1.84838	0.6126	3.81438
O	-0.42336	-0.53011	2.67764
H	-1.38259	-0.40243	2.78168
C	-0.04884	-0.22764	-0.4132
S	-0.13429	-3.3556	0.35599
C	-0.0939	0.99789	-1.29887
C	-0.14023	3.172	-3.08476
C	0.33863	2.26498	-0.89097
C	-0.54675	0.82908	-2.61883
C	-0.5655	1.90762	-3.50388
C	0.31115	3.3479	-1.77553
H	0.70464	2.41143	0.12019
H	-0.87936	-0.14934	-2.9553
H	-0.91461	1.75797	-4.52174
H	0.64522	4.32555	-1.43922
H	-0.16055	4.01153	-3.77354

H at the Midpoint Total Energy = -1324.14825663

H	3.58039	-2.37887	-1.31654
C	2.52159	-2.40329	-1.07251
C	-0.19877	-2.45989	-0.46526
C	1.8397	-1.1933	-0.82413
C	1.85091	-3.6133	-1.01109
C	0.47774	-3.64305	-0.70077
C	0.45254	-1.19722	-0.52636
H	2.38772	-4.53688	-1.20748
H	-0.05141	-4.5901	-0.65499
H	-1.2587	-2.4845	-0.2371
H	3.2586	2.97147	-1.03029
C	2.2019	2.84649	-0.80888
C	-0.51394	2.51748	-0.28096
C	1.38414	3.95721	-0.67374
C	1.67018	1.54887	-0.67538
C	0.29253	1.35569	-0.39839
C	0.01334	3.79031	-0.41338
H	1.80525	4.95242	-0.78219
H	-0.63499	4.65653	-0.32308
H	-1.57435	2.40022	-0.09065
C	0.2362	-0.28141	2.7468
H	-0.03713	-0.13063	1.27964
C	-0.72993	-1.23294	3.38983
H	-0.31315	-1.55173	4.35776
H	-0.89685	-2.1259	2.77826

H	-1.69229	-0.75525	3.58593
C	0.37061	1.12222	3.25182
H	-0.60481	1.60955	3.32643
H	1.02858	1.71174	2.60803
H	0.81731	1.09346	4.25704
O	1.41355	-0.79024	2.29364
H	1.3977	-1.76222	2.24601
C	-0.31045	0.02016	-0.18752
S	2.8161	0.24991	-0.9325
C	-1.80324	-0.05473	-0.42064
C	-4.55304	-0.12097	-1.01438
C	-2.75524	0.12808	0.58894
C	-2.24508	-0.26643	-1.73815
C	-3.60901	-0.29529	-2.03104
C	-4.12237	0.08999	0.29665
H	-2.43288	0.30654	1.60976
H	-1.52004	-0.40286	-2.53616
H	-3.93253	-0.45573	-3.05569
H	-4.84689	0.22799	1.09448
H	-5.61436	-0.14904	-1.24342

DAD = 3.1 Å

H in Acceptor Well Total Energy = -1324.14971169

H	-2.80892	-3.83049	0.83552
C	-2.73396	-2.78774	0.53848
C	-2.53953	-0.11902	-0.24623
C	-1.46866	-2.24329	0.23339
C	-3.87382	-2.0056	0.455
C	-3.77588	-0.65711	0.06161
C	-1.34715	-0.89083	-0.17868
H	-4.84215	-2.43851	0.68879
H	-4.6685	-0.04286	-0.00877
H	-2.46794	0.91725	-0.5576
H	2.49359	-4.16264	0.06076
C	2.46547	-3.1164	-0.23225
C	2.37779	-0.44455	-1.01942
C	3.61576	-2.49057	-0.68619
C	1.24988	-2.40854	-0.16067
C	1.18122	-1.04568	-0.54892
C	3.56964	-1.14465	-1.08796
H	4.54627	-3.0481	-0.74058
H	4.46454	-0.65436	-1.45895
H	2.3508	0.5901	-1.34074
C	0.23216	0.66135	2.5094

H	0.05714	0.10752	0.68986
C	-0.51611	1.93515	2.76493
H	-0.63727	2.05619	3.85282
H	-1.51141	1.92876	2.30857
H	0.03568	2.80252	2.3959
C	1.70044	0.57165	2.78332
H	2.24004	1.39337	2.30577
H	2.10736	-0.38392	2.44299
H	1.86219	0.6418	3.86984
O	-0.41759	-0.51308	2.73064
H	-1.37869	-0.38733	2.81969
C	-0.05191	-0.23753	-0.44378
S	-0.12447	-3.34805	0.38136
C	-0.09696	0.988	-1.32945
C	-0.15047	3.16638	-3.10799
C	0.30474	2.26069	-0.90867
C	-0.52401	0.81481	-2.65726
C	-0.54634	1.89634	-3.53866
C	0.27447	3.34581	-1.79038
H	0.64807	2.40813	0.11047
H	-0.83372	-0.16809	-3.00261
H	-0.87501	1.7444	-4.56298
H	0.58553	4.32807	-1.4454
H	-0.1732	4.00773	-3.79452

H in Donor WellTotal Energy = -1324.15032218

H	-2.81035	-3.835	0.8207
C	-2.73539	-2.79225	0.52366
C	-2.54095	-0.12353	-0.26105
C	-1.47009	-2.2478	0.21858
C	-3.87525	-2.01011	0.44018
C	-3.7773	-0.66163	0.04679
C	-1.34858	-0.89534	-0.1935
H	-4.84357	-2.44302	0.67397
H	-4.66993	-0.04737	-0.02359
H	-2.46937	0.91274	-0.57242
H	2.49217	-4.16715	0.04594
C	2.46404	-3.12091	-0.24707
C	2.37637	-0.44906	-1.03424
C	3.61434	-2.49508	-0.70101
C	1.24845	-2.41305	-0.17549
C	1.17979	-1.05019	-0.56374
C	3.56821	-1.14916	-1.10278
H	4.54484	-3.05261	-0.7554
H	4.46311	-0.65887	-1.47377
H	2.34938	0.58559	-1.35556

C	0.23073	0.65684	2.49458
H	0.12169	0.31179	1.36094
C	-0.51754	1.93064	2.75011
H	-0.6387	2.05168	3.838
H	-1.51283	1.92425	2.29375
H	0.03426	2.79801	2.38109
C	1.69902	0.56714	2.7685
H	2.23861	1.38886	2.29095
H	2.10593	-0.38843	2.42817
H	1.86076	0.63729	3.85502
O	-0.41902	-0.51759	2.71583
H	-1.38012	-0.39184	2.80487
C	-0.05333	-0.24204	-0.4586
S	-0.1259	-3.35256	0.36654
C	-0.09839	0.98349	-1.34427
C	-0.1519	3.16187	-3.12281
C	0.30331	2.25618	-0.92349
C	-0.52544	0.8103	-2.67208
C	-0.54776	1.89183	-3.55348
C	0.27305	3.3413	-1.8052
H	0.64665	2.40362	0.09565
H	-0.83515	-0.1726	-3.01742
H	-0.87643	1.73989	-4.5778
H	0.58411	4.32356	-1.46021
H	-0.17463	4.00322	-3.80934

H at the Midpoint Total Energy = -1324.14377177

H	3.57081	-2.35065	-1.37874
C	2.51191	-2.38024	-1.13576
C	-0.21007	-2.4493	-0.53438
C	1.82828	-1.17539	-0.86843
C	1.84183	-3.59163	-1.09653
C	0.46795	-3.62734	-0.79004
C	0.44079	-1.18555	-0.57099
H	2.37937	-4.51136	-1.30836
H	-0.06075	-4.57538	-0.76281
H	-1.27006	-2.47879	-0.30744
H	3.23504	2.99678	-1.03312
C	2.17995	2.86554	-0.80771
C	-0.53253	2.52156	-0.26897
C	1.35881	3.97171	-0.65595

C	1.65325	1.5649	-0.68621
C	0.27721	1.36386	-0.40526
C	-0.01002	3.79741	-0.3895
H	1.77589	4.96955	-0.75587
H	-0.66043	4.66051	-0.28518
H	-1.5912	2.39794	-0.07299
C	0.30483	-0.33197	2.80277
H	-0.00768	-0.15314	1.29517
C	-0.65037	-1.29168	3.44645
H	-0.22562	-1.6126	4.41052
H	-0.81756	-2.18293	2.83274
H	-1.61331	-0.81863	3.65129
C	0.44552	1.06532	3.31922
H	-0.52927	1.55165	3.40705
H	1.09773	1.66009	2.67471
H	0.90064	1.02778	4.32075
O	1.4697	-0.83022	2.30756
H	1.44845	-1.80035	2.23105
C	-0.32019	0.02569	-0.21243
S	2.80192	0.27151	-0.95642
C	-1.81721	-0.04756	-0.41715
C	-4.57799	-0.1171	-0.95071
C	-2.74648	0.08533	0.62062
C	-2.28599	-0.21235	-1.73189
C	-3.65609	-0.24301	-1.99448
C	-4.11949	0.04645	0.35768
H	-2.4001	0.22484	1.63985
H	-1.57818	-0.311	-2.55075
H	-4.00172	-0.36669	-3.01701
H	-4.82698	0.14657	1.17624
H	-5.64399	-0.14604	-1.1569

DAD = 3.2 Å

H in Acceptor Well Total Energy = -1324.14795498

H	-2.79681	-3.82846	0.86492
C	-2.72655	-2.79124	0.54799
C	-2.5441	-0.13762	-0.29144
C	-1.4637	-2.24618	0.23476
C	-3.87043	-2.01728	0.44428
C	-3.77836	-0.67717	0.02194
C	-1.34734	-0.90039	-0.20151
H	-4.83733	-2.45061	0.68316
H	-4.67445	-0.07026	-0.06638
H	-2.47805	0.89231	-0.62399
H	2.50087	-4.16246	0.05762
C	2.46846	-3.11986	-0.24762

C	2.37004	-0.45686	-1.06533
C	3.61306	-2.49824	-0.72154
C	1.25316	-2.41229	-0.17215
C	1.17869	-1.05422	-0.57676
C	3.56154	-1.15685	-1.1381
H	4.54348	-3.05556	-0.77965
H	4.45226	-0.67015	-1.52362
H	2.33843	0.57442	-1.39695
C	0.23894	0.67749	2.57409
H	0.05384	0.09176	0.64975
C	-0.50956	1.94947	2.83047
H	-0.62319	2.07264	3.91919
H	-1.50762	1.94212	2.38083
H	0.04013	2.81648	2.45701
C	1.70648	0.58732	2.84515
H	2.24593	1.4078	2.36529
H	2.11225	-0.36953	2.50812
H	1.869	0.66193	3.93165
O	-0.41131	-0.50084	2.77192
H	-1.3734	-0.37669	2.85073
C	-0.05428	-0.25039	-0.47435
S	-0.1138	-3.34134	0.40434
C	-0.09819	0.98283	-1.34935
C	-0.15694	3.18154	-3.10266
C	0.26547	2.25865	-0.90378
C	-0.49057	0.81715	-2.68889
C	-0.51625	1.90903	-3.55753
C	0.23353	3.35341	-1.77337
H	0.57955	2.39879	0.12583
H	-0.77118	-0.16779	-3.05296
H	-0.81837	1.76307	-4.59085
H	0.51612	4.33759	-1.40981
H	-0.18129	4.03067	-3.77949

H in Donor WellTotal Energy = -1324.14768111

H	-2.79844	-3.83361	0.84798
C	-2.72818	-2.7964	0.53106
C	-2.54573	-0.14278	-0.30837
C	-1.46532	-2.25134	0.21783
C	-3.87206	-2.02244	0.42734
C	-3.77999	-0.68232	0.00501
C	-1.34897	-0.90555	-0.21845
H	-4.83896	-2.45576	0.66622
H	-4.67608	-0.07542	-0.08332
H	-2.47968	0.88716	-0.64093
H	2.49924	-4.16762	0.04069

C	2.46683	-3.12502	-0.26456
C	2.36842	-0.46202	-1.08227
C	3.61143	-2.50339	-0.73848
C	1.25153	-2.41745	-0.18908
C	1.17706	-1.05938	-0.5937
C	3.55992	-1.16201	-1.15503
H	4.54185	-3.06071	-0.79659
H	4.45063	-0.6753	-1.54055
H	2.33681	0.56927	-1.41388
C	0.23732	0.67233	2.55715
H	0.12919	0.33018	1.43304
C	-0.51119	1.94432	2.81353
H	-0.62482	2.06749	3.90226
H	-1.50925	1.93696	2.3639
H	0.0385	2.81132	2.44007
C	1.70485	0.58217	2.82822
H	2.24431	1.40265	2.34835
H	2.11062	-0.37469	2.49118
H	1.86737	0.65678	3.91472
O	-0.41294	-0.506	2.75498
H	-1.37503	-0.38185	2.8338
C	-0.05591	-0.25554	-0.49129
S	-0.11543	-3.34649	0.3874
C	-0.09982	0.97767	-1.36629
C	-0.15857	3.17639	-3.1196
C	0.26384	2.2535	-0.92072
C	-0.4922	0.812	-2.70583
C	-0.51788	1.90388	-3.57447
C	0.2319	3.34825	-1.79031
H	0.57792	2.39364	0.1089
H	-0.77281	-0.17295	-3.0699
H	-0.82	1.75792	-4.60779
H	0.5145	4.33244	-1.42675
H	-0.18292	4.02552	-3.79643

H at the Midpoint Total Energy = -1324.13811796

H	3.56064	-2.33194	-1.42855
C	2.49942	-2.36239	-1.19601
C	-0.22976	-2.43234	-0.62478
C	1.81849	-1.16133	-0.90656
C	1.82274	-3.57084	-1.19452
C	0.44525	-3.60653	-0.9047
C	0.4282	-1.17171	-0.62016
H	2.35756	-4.48781	-1.42443
H	-0.08884	-4.55196	-0.90928
H	-1.29214	-2.46284	-0.40995

H	3.23367	3.01095	-1.00972
C	2.17778	2.87785	-0.78918
C	-0.53716	2.52987	-0.26199
C	1.35634	3.98268	-0.62881
C	1.64977	1.57658	-0.6833
C	0.27232	1.37323	-0.40968
C	-0.01342	3.80638	-0.36769
H	1.774	4.98135	-0.71746
H	-0.66344	4.66883	-0.25573
H	-1.59616	2.40423	-0.069
C	0.3498	-0.39434	2.85828
H	0.01213	-0.17963	1.30912
C	-0.6003	-1.3627	3.4935
H	-0.16874	-1.69619	4.45055
H	-0.77268	-2.24557	2.86965
H	-1.56116	-0.8914	3.71248
C	0.49982	0.99246	3.39637
H	-0.47231	1.48091	3.50059
H	1.1504	1.59537	2.75836
H	0.961	0.93475	4.39459
O	1.49971	-0.88276	2.32015
H	1.47057	-1.85002	2.21612
C	-0.32553	0.03508	-0.24002
S	2.79843	0.28361	-0.95326
C	-1.82632	-0.03125	-0.41785
C	-4.5977	-0.09425	-0.89469
C	-2.73351	0.04341	0.64514
C	-2.32274	-0.13517	-1.72878
C	-3.69813	-0.16344	-1.963
C	-4.11162	0.00879	0.40997
H	-2.36362	0.13345	1.66173
H	-1.63223	-0.1889	-2.56647
H	-4.06529	-0.2403	-2.98263
H	-4.80179	0.06466	1.24735
H	-5.66778	-0.12025	-1.079

DAD = 3.3 Å

H in Acceptor Well Total Energy = -1324.14640487

H	-2.78552	-3.81035	0.91844
C	-2.71924	-2.7812	0.5754
C	-2.54669	-0.14975	-0.33475
C	-1.4582	-2.23778	0.25315
C	-3.86694	-2.0167	0.4444
C	-3.77963	-0.68852	-0.01455
C	-1.34613	-0.90246	-0.2162
H	-4.83289	-2.44889	0.68911

H	-4.67868	-0.08966	-0.12526
H	-2.48542	0.87149	-0.69374
H	2.50867	-4.15228	0.09231
C	2.47283	-3.11567	-0.23238
C	2.36599	-0.46804	-1.09921
C	3.61321	-2.50183	-0.72654
C	1.25768	-2.40787	-0.1613
C	1.17833	-1.05791	-0.59239
C	3.55763	-1.16817	-1.16698
H	4.54368	-3.0594	-0.7814
H	4.4455	-0.68766	-1.56658
H	2.33132	0.55741	-1.44833
C	0.24805	0.70055	2.64481
H	0.05287	0.08293	0.61569
C	-0.50232	1.97334	2.88449
H	-0.6096	2.11555	3.97178
H	-1.50291	1.95545	2.44106
H	0.04336	2.83485	2.49262
C	1.71397	0.61336	2.91725
H	2.25325	1.42825	2.42792
H	2.12005	-0.34763	2.59355
H	1.87534	0.70308	4.00308
O	-0.4022	-0.47778	2.84264
H	-1.36558	-0.35382	2.90563
C	-0.05434	-0.25633	-0.4989
S	-0.10259	-3.32134	0.45404
C	-0.0994	0.96921	-1.38457
C	-0.1708	3.16072	-3.14446
C	0.22221	2.25401	-0.93372
C	-0.45799	0.78955	-2.73181
C	-0.4902	1.87902	-3.60356
C	0.1851	3.34552	-1.80724
H	0.50563	2.40125	0.1039
H	-0.70789	-0.20245	-3.09929
H	-0.766	1.72383	-4.64289
H	0.4361	4.33709	-1.4406
H	-0.19959	4.00707	-3.8246

H in Donor WellTotal Energy = -1324.14693412

H	-2.78747	-3.81654	0.89811
C	-2.7212	-2.78738	0.55507
C	-2.54865	-0.15594	-0.35508
C	-1.46015	-2.24396	0.23283
C	-3.86889	-2.02289	0.42408
C	-3.78159	-0.6947	-0.03487
C	-1.34809	-0.90864	-0.23653

H	-4.83485	-2.45508	0.66878
H	-4.68063	-0.09585	-0.14558
H	-2.48737	0.8653	-0.71406
H	2.50671	-4.15847	0.07199
C	2.47087	-3.12186	-0.25271
C	2.36403	-0.47423	-1.11953
C	3.61126	-2.50801	-0.74686
C	1.25572	-2.41406	-0.18163
C	1.17637	-1.0641	-0.61271
C	3.55567	-1.17436	-1.18731
H	4.54173	-3.06559	-0.80173
H	4.44355	-0.69384	-1.5869
H	2.32937	0.55122	-1.46865
C	0.24609	0.69436	2.62449
H	0.13888	0.35511	1.5099
C	-0.50427	1.96715	2.86416
H	-0.61156	2.10936	3.95146
H	-1.50486	1.94926	2.42074
H	0.04141	2.82867	2.4723
C	1.71201	0.60717	2.89693
H	2.25129	1.42206	2.40759
H	2.11809	-0.35382	2.57323
H	1.87338	0.69689	3.98275
O	-0.40416	-0.48396	2.82232
H	-1.36753	-0.36001	2.88531
C	-0.0563	-0.26251	-0.51922
S	-0.10454	-3.32753	0.43372
C	-0.10135	0.96302	-1.40489
C	-0.17276	3.15453	-3.16479
C	0.22025	2.24783	-0.95405
C	-0.45994	0.78337	-2.75213
C	-0.49215	1.87283	-3.62388
C	0.18315	3.33933	-1.82757
H	0.50367	2.39506	0.08358
H	-0.70984	-0.20864	-3.11961
H	-0.76796	1.71765	-4.66321
H	0.43414	4.33091	-1.46092
H	-0.20154	4.00089	-3.84492

H at the Midpoint Total Energy = -1324.13323190

H	3.51854	-2.31464	-1.53178
C	2.45938	-2.3455	-1.29003
C	-0.26606	-2.41476	-0.69856
C	1.78672	-1.14834	-0.96796
C	1.77605	-3.55024	-1.31183
C	0.40064	-3.58508	-1.01288

C	0.39901	-1.1583	-0.66783
H	2.3038	-4.46429	-1.56821
H	-0.13884	-4.52719	-1.03669
H	-1.32659	-2.44598	-0.47525
H	3.20832	3.02309	-1.04171
C	2.15566	2.88866	-0.80699
C	-0.55196	2.53806	-0.24253
C	1.33754	3.99251	-0.6235
C	1.6279	1.58715	-0.70617
C	0.25382	1.38216	-0.41565
C	-0.02826	3.81496	-0.34279
H	1.75475	4.99167	-0.70879
H	-0.67516	4.67696	-0.21098
H	-1.60782	2.41145	-0.03333
C	0.46373	-0.44715	2.908
H	0.06095	-0.20143	1.3269
C	-0.47416	-1.42319	3.5469
H	-0.02745	-1.76791	4.49324
H	-0.65643	-2.29845	2.91538
H	-1.43121	-0.95415	3.7869
C	0.63171	0.92897	3.46372
H	-0.33593	1.41882	3.59802
H	1.27097	1.53947	2.82197
H	1.1137	0.85258	4.45111
O	1.59398	-0.92786	2.3233
H	1.55235	-1.89144	2.19216
C	-0.34183	0.04429	-0.2542
S	2.77202	0.29412	-0.99333
C	-1.84685	-0.01645	-0.3942
C	-4.62991	-0.08082	-0.78852
C	-2.72041	-0.00064	0.69853
C	-2.38134	-0.06387	-1.69342
C	-3.76336	-0.09332	-1.886
C	-4.10492	-0.0348	0.50425
H	-2.31656	0.04147	1.70541
H	-1.71688	-0.07371	-2.55363
H	-4.16156	-0.12647	-2.8963
H	-4.76949	-0.02366	1.36383
H	-5.70492	-0.10675	-0.9415

DAD = 3.5 Å

H in Acceptor Well Total Energy = -1324.14346058

H	-2.77839	-3.83939	0.86981
C	-2.71707	-2.81402	0.51475
C	-2.55635	-0.19224	-0.42712
C	-1.45739	-2.26149	0.2055

C	-3.87053	-2.06379	0.35267
C	-3.78872	-0.741	-0.12214
C	-1.35018	-0.93032	-0.2781
H	-4.83616	-2.5034	0.58516
H	-4.69196	-0.1534	-0.25671
H	-2.50021	0.82545	-0.79638
H	2.52265	-4.15234	0.0806
C	2.48038	-3.11991	-0.2564
C	2.35803	-0.48238	-1.15508
C	3.61619	-2.50563	-0.76083
C	1.26206	-2.41783	-0.19168
C	1.17421	-1.07327	-0.6392
C	3.55278	-1.1772	-1.21661
H	4.54942	-3.05894	-0.81186
H	4.43762	-0.69699	-1.62326
H	2.31738	0.53923	-1.51442
C	0.25932	0.73039	2.77705
H	0.04582	0.05477	0.5574
C	-0.49456	2.00228	2.99607
H	-0.59875	2.16259	4.08157
H	-1.49586	1.97312	2.55541
H	0.04849	2.85859	2.58909
C	1.72342	0.64471	3.04573
H	2.2622	1.45429	2.54728
H	2.12725	-0.32063	2.73364
H	1.88539	0.74908	4.13073
O	-0.39123	-0.45148	2.95141
H	-1.35595	-0.32739	2.99252
C	-0.06139	-0.28448	-0.55719
S	-0.0905	-3.32164	0.45251
C	-0.103	0.96382	-1.41064
C	-0.17363	3.20104	-3.11122
C	0.17417	2.24219	-0.91465
C	-0.41834	0.81366	-2.77193
C	-0.45073	1.92602	-3.61432
C	0.13834	3.35599	-1.75926
H	0.42029	2.36348	0.13573
H	-0.63523	-0.17294	-3.17367
H	-0.69336	1.79377	-4.66507
H	0.35559	4.34233	-1.3584
H	-0.20153	4.0653	-3.76851

H in Donor WellTotal Energy = -1324.14334430

H	-2.78075	-3.84686	0.84525
C	-2.71943	-2.82149	0.4902
C	-2.55871	-0.19971	-0.45168

C	-1.45975	-2.26897	0.18095
C	-3.87289	-2.07127	0.32811
C	-3.79108	-0.74848	-0.1467
C	-1.35254	-0.9378	-0.30266
H	-4.83852	-2.51088	0.56061
H	-4.69432	-0.16088	-0.28127
H	-2.50257	0.81797	-0.82093
H	2.52029	-4.15981	0.05604
C	2.47802	-3.12739	-0.28096
C	2.35567	-0.48985	-1.17964
C	3.61383	-2.5131	-0.78538
C	1.2597	-2.42531	-0.21624
C	1.17185	-1.08074	-0.66375
C	3.55041	-1.18467	-1.24116
H	4.54706	-3.06642	-0.83642
H	4.43525	-0.70446	-1.64781
H	2.31502	0.53176	-1.53898
C	0.25696	0.72291	2.7525
H	0.14975	0.38365	1.63791
C	-0.49692	1.99481	2.97151
H	-0.60111	2.15512	4.05702
H	-1.49822	1.96565	2.53086
H	0.04613	2.85111	2.56454
C	1.72106	0.63724	3.02117
H	2.25984	1.44681	2.52272
H	2.12489	-0.32811	2.70909
H	1.88303	0.74161	4.10617
O	-0.3936	-0.45895	2.92685
H	-1.35831	-0.33486	2.96796
C	-0.06376	-0.29196	-0.58174
S	-0.09286	-3.32912	0.42795
C	-0.10536	0.95634	-1.4352
C	-0.17599	3.19357	-3.13577
C	0.1718	2.23471	-0.93921
C	-0.4207	0.80619	-2.79648
C	-0.45309	1.91855	-3.63888
C	0.13598	3.34851	-1.78382
H	0.41793	2.35601	0.11117
H	-0.63759	-0.18042	-3.19822
H	-0.69572	1.78629	-4.68962
H	0.35323	4.33485	-1.38295
H	-0.20389	4.05783	-3.79307

H at the Midpoint Total Energy = -1324.12251805

H	3.47836	-2.33096	-1.61687
C	2.41727	-2.35083	-1.38255

C	-0.31365	-2.39052	-0.81051
C	1.76201	-1.15267	-1.03215
C	1.71334	-3.54255	-1.44455
C	0.33568	-3.56197	-1.15541
C	0.37217	-1.14696	-0.73944
H	2.22696	-4.4576	-1.72494
H	-0.21963	-4.49355	-1.2102
H	-1.37548	-2.41116	-0.59311
H	3.23897	3.00067	-1.0353
C	2.18312	2.87592	-0.8097
C	-0.53364	2.55144	-0.26832
C	1.3757	3.98711	-0.62219
C	1.63962	1.58019	-0.72536
C	0.26065	1.38791	-0.44728
C	0.00576	3.82263	-0.35259
H	1.80451	4.9823	-0.69575
H	-0.63181	4.69098	-0.21698
H	-1.59192	2.43468	-0.06615
C	0.51801	-0.50154	3.03477
H	0.08525	-0.22143	1.36242
C	-0.43968	-1.46857	3.65259
H	-0.00901	-1.82647	4.60196
H	-0.62642	-2.33564	3.01155
H	-1.39221	-0.98688	3.88596
C	0.70481	0.86638	3.59777
H	-0.25542	1.37067	3.73115
H	1.35871	1.46922	2.96424
H	1.17818	0.77387	4.58859
O	1.62907	-0.98771	2.41864
H	1.56193	-1.94615	2.26161
C	-0.34752	0.05867	-0.30993
S	2.77083	0.27369	-0.99868
C	-1.85669	0.01276	-0.40309
C	-4.65061	-0.02899	-0.71028
C	-2.6941	-0.0199	0.71705
C	-2.43219	0.02356	-1.68518
C	-3.81976	0.00476	-1.83461
C	-4.08399	-0.04176	0.56561
H	-2.25473	-0.02635	1.70977
H	-1.79572	0.04996	-2.56611
H	-4.25003	0.01631	-2.83219
H	-4.7207	-0.06758	1.44577
H	-5.7301	-0.04564	-0.8294

Table S5. The atom coordinates and absolute energies of the TRS at different DADs for the reaction of TXn^+ (for Table 1 data in the paper)

DAD = 2.9 Å

H in Acceptor Well Total Energy = -1093.10666143

H	-3.30131	-2.73788	-0.06734
C	-3.05228	-1.7136	-0.33095
C	-2.42565	0.91768	-1.04808
C	-1.70365	-1.338	-0.47784
C	-4.06099	-0.78425	-0.54274
C	-3.74997	0.53901	-0.91197
C	-1.37198	-0.00594	-0.83175
H	-5.09835	-1.08805	-0.43686
H	-4.54549	1.25408	-1.09794
H	-2.17732	1.9347	-1.34397
H	1.99178	-3.77861	-0.72785
C	2.09271	-2.72139	-0.95808
C	2.35111	-0.01073	-1.59903
C	3.30031	-2.22302	-1.42885
C	0.99034	-1.86217	-0.79994
C	1.11053	-0.48563	-1.11147
C	3.43138	-0.86192	-1.75956
H	4.14297	-2.89634	-1.55592
H	4.37332	-0.48271	-2.14362
H	2.44475	1.04209	-1.85539
C	0.27426	1.28833	1.8465
H	0.12398	0.81279	0.28417
C	0.17617	2.7882	1.88798
H	0.14997	3.11325	2.93863
H	-0.72866	3.1574	1.39297
H	1.04862	3.25055	1.41854
C	1.53067	0.61534	2.31448
H	2.41029	1.05034	1.83314
H	1.50053	-0.46011	2.12345
H	1.62563	0.76632	3.3998
O	-0.83994	0.56717	2.11121
H	-1.65028	1.10441	2.06445
C	0.00852	0.44744	-0.91616
H	0.13145	1.39283	-1.44377
S	-0.50342	-2.59158	-0.22625

H in Donor Well Total Energy = -1093.10658831

H	-3.3023	-2.74103	-0.07768
C	-3.05328	-1.71675	-0.34129

C	-2.42665	0.91453	-1.05843
C	-1.70464	-1.34115	-0.48818
C	-4.06199	-0.7874	-0.55308
C	-3.75096	0.53586	-0.92231
C	-1.37298	-0.00908	-0.8421
H	-5.09935	-1.0912	-0.4472
H	-4.54649	1.25093	-1.10829
H	-2.17831	1.93156	-1.35431
H	1.99079	-3.78176	-0.73819
C	2.09171	-2.72454	-0.96842
C	2.35012	-0.01388	-1.60937
C	3.29931	-2.22617	-1.43919
C	0.98935	-1.86532	-0.81028
C	1.10954	-0.48878	-1.12181
C	3.43039	-0.86507	-1.76991
H	4.14197	-2.89949	-1.56626
H	4.37232	-0.48586	-2.15397
H	2.44376	1.03895	-1.86574
C	0.27326	1.28518	1.83615
H	0.1578	0.91983	0.63583
C	0.17518	2.78505	1.87764
H	0.14898	3.1101	2.92829
H	-0.72966	3.15425	1.38263
H	1.04762	3.2474	1.40819
C	1.52967	0.61219	2.30413
H	2.4093	1.04719	1.82279
H	1.49954	-0.46326	2.11311
H	1.62464	0.76317	3.38946
O	-0.84094	0.56402	2.10087
H	-1.65128	1.10126	2.05411
C	0.00752	0.44429	-0.9265
H	0.13045	1.38968	-1.45411
S	-0.50441	-2.59473	-0.23659

H at the Midpoint Total Energy = -1093.10593172

H	2.43835	-2.69129	-1.43175
C	2.42289	-1.96208	-0.62635
C	2.3892	-0.11469	1.47523
C	1.21144	-1.34007	-0.27003
C	3.58937	-1.6607	0.06252
C	3.57495	-0.73762	1.12637
C	1.1821	-0.39545	0.78661
H	4.51621	-2.15465	-0.21424
H	4.48723	-0.52424	1.675
H	2.36732	0.59095	2.30295
H	-2.97879	-2.25549	-1.40109

C	-2.83928	-1.52734	-0.60658
C	-2.48944	0.31175	1.47203
C	-3.93698	-1.03011	0.08343
C	-1.54199	-1.10625	-0.26281
C	-1.35156	-0.16801	0.78113
C	-3.764	-0.11111	1.13447
H	-4.93391	-1.36826	-0.18372
H	-4.62539	0.26007	1.68108
H	-2.34835	1.01994	2.28535
C	0.38017	2.58166	-0.64584
H	0.17531	1.45638	0.24538
C	0.86731	3.74318	0.17545
H	1.1457	4.5645	-0.50142
H	1.74459	3.48443	0.77835
H	0.07979	4.11121	0.83853
C	-0.91477	2.69576	-1.39459
H	-1.7181	3.03814	-0.73726
H	-1.19439	1.74397	-1.85271
H	-0.79111	3.43729	-2.19745
O	1.29815	1.82627	-1.29258
H	2.20113	1.97292	-0.96003
C	-0.02954	0.3311	1.13659
H	0.01215	0.81578	2.11158
S	-0.21471	-1.81404	-1.17378

DAD = 3.0 Å

H in Acceptor Well Total Energy = -1093.10427735

H	-3.29484	-2.74105	-0.05067
C	-3.04894	-1.71899	-0.32565
C	-2.43034	0.90642	-1.07205
C	-1.70197	-1.34308	-0.48571
C	-4.06017	-0.79279	-0.5392
C	-3.75304	0.52745	-0.92263
C	-1.374	-0.01402	-0.85502
H	-5.09642	-1.09664	-0.42316
H	-4.55069	1.24007	-1.10902
H	-2.18485	1.92124	-1.37759
H	1.99614	-3.78174	-0.73621
C	2.09413	-2.72627	-0.97551
C	2.34577	-0.01988	-1.63868
C	3.29913	-2.22932	-1.45447
C	0.99108	-1.86771	-0.82024
C	1.1073	-0.49325	-1.14367
C	3.42692	-0.8703	-1.79568
H	4.14262	-2.90208	-1.57912
H	4.36723	-0.4924	-2.185

H	2.43673	1.03121	-1.90282
C	0.2795	1.30797	1.90117
H	0.11731	0.79474	0.21499
C	0.17906	2.80665	1.93799
H	0.14693	3.1341	2.988
H	-0.72333	3.1734	1.43712
H	1.05366	3.26846	1.47228
C	1.53478	0.63518	2.36802
H	2.4111	1.04937	1.8628
H	1.49046	-0.44414	2.20574
H	1.64822	0.81372	3.44773
O	-0.83532	0.58368	2.15451
H	-1.64623	1.11843	2.09062
C	0.0046	0.43808	-0.95675
H	0.12642	1.37894	-1.49265
S	-0.49804	-2.59255	-0.22991

H in Donor WellTotal Energy = -1093.10427796

H	-3.29627	-2.7456	-0.06564
C	-3.05038	-1.72355	-0.34062
C	-2.43178	0.90187	-1.08702
C	-1.70341	-1.34764	-0.50068
C	-4.0616	-0.79735	-0.55417
C	-3.75448	0.5229	-0.9376
C	-1.37544	-0.01858	-0.86999
H	-5.09786	-1.10119	-0.43813
H	-4.55212	1.23551	-1.12399
H	-2.18629	1.91668	-1.39256
H	1.99469	-3.78629	-0.75118
C	2.09269	-2.73082	-0.99048
C	2.34433	-0.02444	-1.65365
C	3.29769	-2.23388	-1.46944
C	0.98964	-1.87227	-0.83521
C	1.10586	-0.4978	-1.15864
C	3.42548	-0.87486	-1.81065
H	4.14118	-2.90663	-1.59408
H	4.36579	-0.49696	-2.19997
H	2.43529	1.02665	-1.91779
C	0.27806	1.30341	1.88619
H	0.16535	0.94676	0.71445
C	0.17762	2.80209	1.92302
H	0.14549	3.12954	2.97303
H	-0.72476	3.16884	1.42215
H	1.05222	3.2639	1.45731

C	1.53334	0.63062	2.35305
H	2.40965	1.04481	1.84783
H	1.48902	-0.44869	2.19077
H	1.64678	0.80916	3.43276
O	-0.83676	0.57913	2.13953
H	-1.64767	1.11387	2.07565
C	0.00316	0.43353	-0.97172
H	0.12498	1.37439	-1.50762
S	-0.49948	-2.59711	-0.24488

H at the Midpoint Total Energy = -1093.10167395

H	2.40795	-2.68491	-1.48617
C	2.39806	-1.97983	-0.65947
C	2.3781	-0.19523	1.49632
C	1.19226	-1.35656	-0.28686
C	3.56591	-1.71079	0.04036
C	3.55822	-0.81915	1.13092
C	1.16958	-0.44367	0.7978
H	4.48845	-2.20548	-0.24915
H	4.47155	-0.63075	1.68692
H	2.36139	0.48703	2.34349
H	-3.00549	-2.19398	-1.45449
C	-2.86006	-1.49004	-0.6395
C	-2.49607	0.28726	1.49037
C	-3.95421	-0.99807	0.05991
C	-1.55929	-1.09471	-0.27941
C	-1.36114	-0.18825	0.79125
C	-3.77421	-0.10974	1.13609
H	-4.95422	-1.3161	-0.2202
H	-4.63333	0.25787	1.68866
H	-2.34942	0.97168	2.32277
C	0.4277	2.63715	-0.62925
H	0.19587	1.45889	0.26961
C	0.92656	3.7724	0.21919
H	1.22528	4.60214	-0.43891
H	1.79323	3.48663	0.82489
H	0.13882	4.14055	0.88175
C	-0.86073	2.78125	-1.38125
H	-1.66956	3.09133	-0.71463
H	-1.1328	1.8506	-1.88434
H	-0.73444	3.55975	-2.14839
O	1.33706	1.87313	-1.27804
H	2.237	1.99006	-0.92584
C	-0.03595	0.28062	1.16846
H	0.00525	0.73793	2.1566

S	-0.23678	-1.78826	-1.20748

DAD = 3.1 Å

H in Acceptor Well Total Energy = -1093.10197109

H	-3.2894	-2.748	-0.04929
C	-3.04703	-1.72952	-0.34023
C	-2.43759	0.88613	-1.12833
C	-1.70176	-1.35257	-0.51099
C	-4.06134	-0.8091	-0.56419
C	-3.75867	0.50592	-0.96853
C	-1.37807	-0.02825	-0.90121
H	-5.09644	-1.11363	-0.43993
H	-4.55876	1.21377	-1.16253
H	-2.19545	1.89733	-1.44806
H	2.00165	-3.78634	-0.74363
C	2.09583	-2.73395	-0.99753
C	2.33802	-0.0358	-1.69813
C	3.29745	-2.24041	-1.4886
C	0.99143	-1.87615	-0.84943
C	1.10256	-0.50564	-1.19187
C	3.42046	-0.88566	-1.84829
H	4.14207	-2.9127	-1.60802
H	4.35831	-0.51074	-2.24632
H	2.42512	1.01196	-1.97622
C	0.28227	1.32227	1.93702
H	0.10908	0.77424	0.13653
C	0.17979	2.8197	1.96836
H	0.14079	3.14926	3.01778
H	-0.71955	3.18416	1.46082
H	1.05708	3.28107	1.50752
C	1.53653	0.64929	2.40199
H	2.40939	1.04315	1.87503
H	1.47898	-0.43286	2.2669
H	1.6674	0.85348	3.47551
O	-0.83308	0.59491	2.17897
H	-1.64374	1.12848	2.1028
C	-0.0018	0.42338	-1.01616
H	0.1189	1.35964	-1.5603
S	-0.49274	-2.594	-0.23924

H in Donor Well Total Energy = -1093.10190816

H	-3.2894	-2.748	-0.04929
C	-3.04703	-1.72952	-0.34023

C	-2.43759	0.88613	-1.12833
C	-1.70176	-1.35257	-0.51099
C	-4.06134	-0.8091	-0.56419
C	-3.75867	0.50592	-0.96853
C	-1.37807	-0.02825	-0.90121
H	-5.09644	-1.11363	-0.43993
H	-4.55876	1.21377	-1.16253
H	-2.19545	1.89733	-1.44806
H	2.00165	-3.78634	-0.74363
C	2.09583	-2.73395	-0.99753
C	2.33802	-0.0358	-1.69813
C	3.29745	-2.24041	-1.4886
C	0.99143	-1.87615	-0.84943
C	1.10256	-0.50564	-1.19187
C	3.42046	-0.88566	-1.84829
H	4.14207	-2.9127	-1.60802
H	4.35831	-0.51074	-2.24632
H	2.42512	1.01196	-1.97622
C	0.28227	1.32227	1.93702
H	0.17139	0.97141	0.78433
C	0.17979	2.8197	1.96836
H	0.14079	3.14926	3.01778
H	-0.71955	3.18416	1.46082
H	1.05708	3.28107	1.50752
C	1.53653	0.64929	2.40199
H	2.40939	1.04315	1.87503
H	1.47898	-0.43286	2.2669
H	1.6674	0.85348	3.47551
O	-0.83308	0.59491	2.17897
H	-1.64374	1.12848	2.1028
C	-0.0018	0.42338	-1.01616
H	0.1189	1.35964	-1.5603
S	-0.49274	-2.594	-0.23924

H at the Midpoint Total Energy = -1093.09662916

H	2.38588	-2.66358	-1.54821
C	2.37916	-1.98768	-0.69744
C	2.36681	-0.27958	1.51985
C	1.17778	-1.3668	-0.30731
C	3.54659	-1.75424	0.01583
C	3.54245	-0.90138	1.13698
C	1.15881	-0.49201	0.8086
H	4.46578	-2.24696	-0.2874
H	4.45528	-0.74087	1.70248
H	2.35313	0.37422	2.38918
H	-3.02402	-2.12756	-1.51508
C	-2.87475	-1.45292	-0.67637

C	-2.50169	0.24843	1.51356
C	-3.96659	-0.97537	0.03669
C	-1.57187	-1.08162	-0.29942
C	-1.36871	-0.21356	0.80199
C	-3.78204	-0.12521	1.1426
H	-4.9685	-1.27508	-0.25648
H	-4.63964	0.2313	1.70471
H	-2.35134	0.90339	2.36863
C	0.46538	2.69346	-0.60849
H	0.21186	1.46029	0.29567
C	0.9723	3.80266	0.26702
H	1.28757	4.64132	-0.37225
H	1.8297	3.49273	0.87369
H	0.18397	4.1683	0.93013
C	-0.81869	2.86229	-1.36012
H	-1.63299	3.13777	-0.68502
H	-1.08084	1.95334	-1.90573
H	-0.69359	3.67575	-2.09078
O	1.36753	1.92496	-1.26205
H	2.26457	2.01898	-0.89579
C	-0.04165	0.22713	1.19984
H	-0.0012	0.65615	2.20061
S	-0.25187	-1.75064	-1.24832

DAD = 3.2 Å

H in Acceptor Well Total Energy = -1093.09990303

H	-3.27278	-2.76327	-0.03603
C	-3.03909	-1.74963	-0.35011
C	-2.45201	0.85238	-1.19986
C	-1.69709	-1.3621	-0.52049
C	-4.06153	-0.84627	-0.60525
C	-3.76994	0.46111	-1.04105
C	-1.3844	-0.04392	-0.94074
H	-5.09423	-1.15901	-0.48134
H	-4.57617	1.15484	-1.25918
H	-2.21843	1.85833	-1.54161
H	2.02974	-3.76635	-0.68794
C	2.11373	-2.71955	-0.96722
C	2.33017	-0.03653	-1.73331
C	3.31006	-2.22664	-1.47202
C	1.00172	-1.86878	-0.83909
C	1.09952	-0.50568	-1.21447
C	3.42006	-0.87979	-1.86449
H	4.16081	-2.89368	-1.57649
H	4.35405	-0.506	-2.27254
H	2.40722	1.00515	-2.03593

C	0.28051	1.34357	1.98742
H	0.09633	0.76074	0.07262
C	0.17896	2.84009	2.01182
H	0.14432	3.17391	3.06033
H	-0.72181	3.2028	1.50592
H	1.05501	3.29855	1.54597
C	1.53591	0.66928	2.44391
H	2.40446	1.05446	1.90368
H	1.47122	-0.4136	2.31975
H	1.68005	0.88344	3.51409
O	-0.83484	0.61621	2.22937
H	-1.64433	1.15147	2.15235
C	-0.01272	0.41569	-1.06102
H	0.10571	1.34254	-1.62153
S	-0.4753	-2.58151	-0.20669

H in Donor WellTotal Energy = -1093.10025702

H	-3.27278	-2.76327	-0.03603
C	-3.03909	-1.74963	-0.35011
C	-2.45201	0.85238	-1.19986
C	-1.69709	-1.3621	-0.52049
C	-4.06153	-0.84627	-0.60525
C	-3.76994	0.46111	-1.04105
C	-1.3844	-0.04392	-0.94074
H	-5.09423	-1.15901	-0.48134
H	-4.57617	1.15484	-1.25918
H	-2.21843	1.85833	-1.54161
H	2.02974	-3.76635	-0.68794
C	2.11373	-2.71955	-0.96722
C	2.33017	-0.03653	-1.73331
C	3.31006	-2.22664	-1.47202
C	1.00172	-1.86878	-0.83909
C	1.09952	-0.50568	-1.21447
C	3.42006	-0.87979	-1.86449
H	4.16081	-2.89368	-1.57649
H	4.35405	-0.506	-2.27254
H	2.40722	1.00515	-2.03593
C	0.28051	1.34357	1.98742
H	0.17147	0.99851	0.85378
C	0.17896	2.84009	2.01182
H	0.14432	3.17391	3.06033
H	-0.72181	3.2028	1.50592
H	1.05501	3.29855	1.54597
C	1.53591	0.66928	2.44391
H	2.40446	1.05446	1.90368
H	1.47122	-0.4136	2.31975

H	1.68005	0.88344	3.51409
O	-0.83484	0.61621	2.22937
H	-1.64433	1.15147	2.15235
C	-0.01272	0.41569	-1.06102
H	0.10571	1.34254	-1.62153
S	-0.4753	-2.58151	-0.20669

H at the Midpoint Total Energy = -1093.09149325

H	2.40601	-2.59421	-1.62589
C	2.39366	-1.95653	-0.74617
C	2.36667	-0.34941	1.54592
C	1.18994	-1.35408	-0.33593
C	3.55641	-1.75522	-0.01539
C	3.54456	-0.95405	1.14312
C	1.1635	-0.52909	0.81762
H	4.47769	-2.23388	-0.33441
H	4.45368	-0.81919	1.72117
H	2.34767	0.26609	2.44263
H	-3.00538	-2.08116	-1.58824
C	-2.8609	-1.44461	-0.71947
C	-2.50028	0.15738	1.54679
C	-3.95609	-1.008	0.01463
C	-1.56102	-1.08224	-0.32475
C	-1.36388	-0.26391	0.81541
C	-3.77771	-0.2081	1.15851
H	-4.95588	-1.30105	-0.29227
H	-4.638	0.11629	1.73577
H	-2.35453	0.77409	2.43056
C	0.44393	2.75754	-0.57933
H	0.20142	1.46168	0.32728
C	0.93371	3.8507	0.32379
H	1.2331	4.71098	-0.29451
H	1.79729	3.53958	0.9207
H	0.14058	4.18556	0.9972
C	-0.84614	2.91815	-1.32028
H	-1.66393	3.1521	-0.63394
H	-1.08749	2.02096	-1.89389
H	-0.74403	3.758	-2.02467
O	1.35618	2.01586	-1.24963
H	2.25139	2.11604	-0.88048
C	-0.04109	0.16583	1.23387
H	-0.00871	0.55687	2.25038
S	-0.23436	-1.69311	-1.30267

DAD = 3.3 Å

H in Acceptor Well Total Energy = -1093.09779613

H	-3.26419	-2.77351	-0.03781
C	-3.03524	-1.76315	-0.36568
C	-2.46033	0.82968	-1.25211
C	-1.69519	-1.37032	-0.53778
C	-4.06201	-0.86946	-0.63746
C	-3.77639	0.43291	-1.09178
C	-1.38835	-0.05633	-0.97596
H	-5.09332	-1.18629	-0.51232
H	-4.58587	1.11876	-1.3225
H	-2.23141	1.83214	-1.60696
H	2.04414	-3.75794	-0.66967
C	2.12249	-2.71469	-0.96355
C	2.32475	-0.0411	-1.76725
C	3.31583	-2.22254	-1.47634
C	1.00636	-1.86793	-0.84667
C	1.09665	-0.50941	-1.24104
C	3.41869	-0.8805	-1.88737
H	4.16991	-2.88658	-1.57242
H	4.35062	-0.50766	-2.301
H	2.3962	0.99691	-2.08347
C	0.28197	1.36315	2.04103
H	0.0877	0.74843	0.02143
C	0.18006	2.85857	2.06264
H	0.14784	3.19331	3.11123
H	-0.7218	3.22028	1.55842
H	1.05512	3.31659	1.59472
C	1.53704	0.68726	2.49346
H	2.40569	1.07711	1.95699
H	1.47316	-0.39475	2.36266
H	1.67967	0.89545	3.56534
O	-0.83383	0.63278	2.27156
H	-1.64227	1.1681	2.18832
C	-0.02043	0.40628	-1.10268
H	0.09685	1.32831	-1.67132
S	-0.46625	-2.57641	-0.20013

H in Donor WellTotal Energy = -1093.09795002

H	-3.26419	-2.77351	-0.03781
C	-3.03524	-1.76315	-0.36568
C	-2.46033	0.82968	-1.25211
C	-1.69519	-1.37032	-0.53778
C	-4.06201	-0.86946	-0.63746
C	-3.77639	0.43291	-1.09178
C	-1.38835	-0.05633	-0.97596
H	-5.09332	-1.18629	-0.51232

H	-4.58587	1.11876	-1.3225
H	-2.23141	1.83214	-1.60696
H	2.04414	-3.75794	-0.66967
C	2.12249	-2.71469	-0.96355
C	2.32475	-0.0411	-1.76725
C	3.31583	-2.22254	-1.47634
C	1.00636	-1.86793	-0.84667
C	1.09665	-0.50941	-1.24104
C	3.41869	-0.8805	-1.88737
H	4.16991	-2.88658	-1.57242
H	4.35062	-0.50766	-2.301
H	2.3962	0.99691	-2.08347
C	0.28197	1.36315	2.04103
H	0.17384	1.021	0.91691
C	0.18006	2.85857	2.06264
H	0.14784	3.19331	3.11123
H	-0.7218	3.22028	1.55842
H	1.05512	3.31659	1.59472
C	1.53704	0.68726	2.49346
H	2.40569	1.07711	1.95699
H	1.47316	-0.39475	2.36266
H	1.67967	0.89545	3.56534
O	-0.83383	0.63278	2.27156
H	-1.64227	1.1681	2.18832
C	-0.02043	0.40628	-1.10268
H	0.09685	1.32831	-1.67132
S	-0.46625	-2.57641	-0.20013

H at the Midpoint Total Energy = -1093.08570278

H	2.39919	-2.56222	-1.68704
C	2.38684	-1.95723	-0.7845
C	2.35942	-0.43616	1.56595
C	1.18518	-1.36321	-0.35692
C	3.54757	-1.79035	-0.04175
C	3.53524	-1.03285	1.14576
C	1.15846	-0.58081	0.82624
H	4.46736	-2.26255	-0.3744
H	4.44266	-0.92498	1.73214
H	2.34043	0.14655	2.48429
H	-3.00994	-2.02716	-1.64565
C	-2.86479	-1.4239	-0.75352
C	-2.50288	0.0916	1.57182
C	-3.95971	-1.01159	-0.00494
C	-1.56461	-1.08066	-0.34348
C	-1.36646	-0.30587	0.82686
C	-3.78063	-0.25512	1.16821

H	-4.95994	-1.29002	-0.32381
H	-4.64093	0.05043	1.75566
H	-2.35637	0.67523	2.47762
C	0.45554	2.8158	-0.54343
H	0.20584	1.45809	0.36032
C	0.94317	3.88572	0.38642
H	1.24029	4.7617	-0.21108
H	1.8076	3.56167	0.97478
H	0.14966	4.20244	1.06795
C	-0.83485	2.98854	-1.2795
H	-1.65167	3.21169	-0.5886
H	-1.07662	2.10138	-1.86809
H	-0.73271	3.84068	-1.96945
O	1.36668	2.08119	-1.22296
H	2.25944	2.17018	-0.84595
C	-0.04385	0.10039	1.26408
H	-0.0142	0.45915	2.2925
S	-0.23728	-1.65464	-1.34212

DAD = 3.5 Å

H in Acceptor Well Total Energy = -1093.09367099

H	-3.24084	-2.7818	-0.00244
C	-3.02296	-1.78195	-0.36789
C	-2.47731	0.78212	-1.35226
C	-1.68798	-1.38159	-0.55769
C	-4.05969	-0.90962	-0.67052
C	-3.78859	0.37752	-1.17408
C	-1.39547	-0.08121	-1.04482
H	-5.08736	-1.23229	-0.53109
H	-4.60573	1.04599	-1.42736
H	-2.25928	1.77366	-1.74221
H	2.07641	-3.73474	-0.62043
C	2.14134	-2.70198	-0.95211
C	2.30956	-0.05671	-1.8536
C	3.32556	-2.21595	-1.49166
C	1.01743	-1.86321	-0.85803
C	1.09	-0.51848	-1.3015
C	3.41118	-0.8885	-1.9514
H	4.186	-2.87404	-1.57051
H	4.33636	-0.52128	-2.38458
H	2.36787	0.97049	-2.20517
C	0.28665	1.40091	2.14071
H	0.07315	0.7253	-0.07894
C	0.18108	2.89424	2.15201
H	0.15402	3.23378	3.19973
H	-0.72364	3.25179	1.6508

H	1.05344	3.35061	1.6779
C	1.53822	0.72476	2.59208
H	2.4106	1.13084	2.0745
H	1.48244	-0.35485	2.44175
H	1.6663	0.91579	3.66955
O	-0.82978	0.66468	2.34838
H	-1.63788	1.19658	2.23614
C	-0.03407	0.38604	-1.19353
H	0.07971	1.29322	-1.78626
S	-0.44304	-2.55649	-0.17056

H in Donor WellTotal Energy = -1093.09322662

H	-3.24084	-2.7818	-0.00244
C	-3.02296	-1.78195	-0.36789
C	-2.47731	0.78212	-1.35226
C	-1.68798	-1.38159	-0.55769
C	-4.05969	-0.90962	-0.67052
C	-3.78859	0.37752	-1.17408
C	-1.39547	-0.08121	-1.04482
H	-5.08736	-1.23229	-0.53109
H	-4.60573	1.04599	-1.42736
H	-2.25928	1.77366	-1.74221
H	2.07641	-3.73474	-0.62043
C	2.14134	-2.70198	-0.95211
C	2.30956	-0.05671	-1.8536
C	3.32556	-2.21595	-1.49166
C	1.01743	-1.86321	-0.85803
C	1.09	-0.51848	-1.3015
C	3.41118	-0.8885	-1.9514
H	4.186	-2.87404	-1.57051
H	4.33636	-0.52128	-2.38458
H	2.36787	0.97049	-2.20517
C	0.28665	1.40091	2.14071
H	0.17944	1.06166	1.02612
C	0.18108	2.89424	2.15201
H	0.15402	3.23378	3.19973
H	-0.72364	3.25179	1.6508
H	1.05344	3.35061	1.6779
C	1.53822	0.72476	2.59208
H	2.4106	1.13084	2.0745
H	1.48244	-0.35485	2.44175
H	1.6663	0.91579	3.66955
O	-0.82978	0.66468	2.34838
H	-1.63788	1.19658	2.23614
C	-0.03407	0.38604	-1.19353
H	0.07971	1.29322	-1.78626

S	-0.44304	-2.55649	-0.17056

H at the Midpoint Total Energy = -1093.07379688

H	2.38605	-2.46826	-1.81306
C	2.37215	-1.934	-0.86697
C	2.34056	-0.59825	1.59392
C	1.17385	-1.36071	-0.40446
C	3.52805	-1.83824	-0.10403
C	3.51319	-1.17462	1.13823
C	1.145	-0.67062	0.83521
H	4.44558	-2.29399	-0.4647
H	4.41671	-1.12199	1.73789
H	2.32002	-0.08549	2.55277
H	-3.01934	-1.88285	-1.76692
C	-2.87351	-1.35131	-0.83044
C	-2.51099	-0.02257	1.60708
C	-3.96859	-0.98919	-0.05624
C	-1.57307	-1.05154	-0.38934
C	-1.37386	-0.37059	0.83819
C	-3.78912	-0.32675	1.17249
H	-4.9695	-1.23425	-0.39943
H	-4.64995	-0.06008	1.77773
H	-2.36383	0.49026	2.55444
C	0.49502	2.93524	-0.48735
H	0.22058	1.4597	0.41263
C	0.98244	3.95697	0.49233
H	1.28164	4.85909	-0.0648
H	1.84495	3.60526	1.06675
H	0.18751	4.24349	1.1852
C	-0.78792	3.13918	-1.22206
H	-1.60356	3.36256	-0.53021
H	-1.04007	2.26829	-1.8297
H	-0.66908	4.0044	-1.89372
O	1.40229	2.2057	-1.17743
H	2.28703	2.25588	-0.77338
C	-0.05385	-0.01584	1.31261
H	-0.03312	0.27526	2.3624
S	-0.24282	-1.54981	-1.42299

Table S6. The atom coordinates and absolute energies of the TRS at different DADs for the reaction of $PhXn^+$ (for Figure 1 in the paper) (The geometry of the $PhXn^+$ reaction is further refined to obtain the symmetrical double potential wells (fitted to the 6^{th}-order polynomial) so that the small barrier difference at the bottom of the double potential wells from that of the reaction of Xn^+ can be clearly recognized. Note that the 2° KIEs calculated from the refined geometries are the same as the ones in Table 1 in the paper within the calculation error.)

DAD = 2.9 Å

H in Donor WellTotal Energy = -1001.190348

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.25000000
H	4.63173015	0.00000000	3.20871324
C	3.73754858	0.60855564	3.11958772
C	1.38349790	2.11974999	2.90228217
C	2.48689357	-0.02398662	3.10021488
C	3.79728683	1.99070783	3.02782038
C	2.61498392	2.75208706	2.91658457
C	1.28298139	0.70862896	3.00224389
H	4.76255838	2.48819696	3.04606839
H	2.67085814	3.83427823	2.84933083
H	0.47225470	2.70479733	2.82507993
H	2.45484066	-3.88686707	3.54478066
C	1.46143679	-3.45651299	3.46856990
C	-1.07320589	-2.26738131	3.30272489
C	0.31533013	-4.22998715	3.58467085
C	1.33354381	-2.07914825	3.26139294
C	0.07317415	-1.44963530	3.16266750
C	-0.95716988	-3.63250163	3.50816968
H	0.40456997	-5.29969925	3.74940582
H	-1.84948570	-4.24086989	3.61899076
H	-2.05565111	-1.80962626	3.26005514
C	-0.55156119	1.29144822	-0.53064326
H	-0.27057564	1.38323174	-1.59088398
H	-0.15190995	2.15789297	0.00658628
H	-1.64174368	1.31477614	-0.47200710
C	-0.60244598	-1.31060746	-0.40756781
H	-1.68931428	-1.30094947	-0.29460150
H	-0.17868217	-2.13675043	0.16961080
H	-0.36932019	-1.48617132	-1.46802218
O	1.34363037	-0.08293827	0.18919447
H	1.77780678	0.78594146	0.13082375
C	-0.00000057	-0.00000045	2.89999946
O	2.50175341	-1.37656955	3.19753193
C	-1.24396285	0.72269961	3.33984095
C	-3.57096194	1.97726718	4.30642619
C	-2.41922938	0.73628071	2.57627546

C	-1.25213668	1.33989502	4.60283475
C	-2.40812385	1.95910323	5.08131152
C	-3.57358255	1.36288767	3.05198494
H	-2.43672974	0.25212733	1.60446338
H	-0.35746066	1.32431010	5.21898875
H	-2.39658880	2.42768244	6.06131552
H	-4.47302147	1.36877209	2.44258023
H	-4.46781993	2.46452204	4.67769675

H in Acceptor Well Total Energy =-1001.1906012

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.65000000
H	4.63173015	0.00000000	3.20871324
C	3.73754858	0.60855564	3.11958772
C	1.38349790	2.11974999	2.90228217
C	2.48689357	-0.02398662	3.10021488
C	3.79728683	1.99070783	3.02782038
C	2.61498392	2.75208706	2.91658457
C	1.28298139	0.70862896	3.00224389
H	4.76255838	2.48819696	3.04606839
H	2.67085814	3.83427823	2.84933083
H	0.47225470	2.70479733	2.82507993
H	2.45484066	-3.88686707	3.54478066
C	1.46143679	-3.45651299	3.46856990
C	-1.07320589	-2.26738131	3.30272489
C	0.31533013	-4.22998715	3.58467085
C	1.33354381	-2.07914825	3.26139294
C	0.07317415	-1.44963530	3.16266750
C	-0.95716988	-3.63250163	3.50816968
H	0.40456997	-5.29969925	3.74940582
H	-1.84948570	-4.24086989	3.61899076
H	-2.05565111	-1.80962626	3.26005514
C	-0.55156119	1.29144822	-0.53064326
H	-0.27057564	1.38323174	-1.59088398
H	-0.15190995	2.15789297	0.00658628
H	-1.64174368	1.31477614	-0.47200710
C	-0.60244598	-1.31060746	-0.40756781
H	-1.68931428	-1.30094947	-0.29460150
H	-0.17868217	-2.13675043	0.16961080
H	-0.36932019	-1.48617132	-1.46802218
O	1.34363037	-0.08293827	0.18919447
H	1.77780678	0.78594146	0.13082375
C	-0.00000057	-0.00000045	2.89999946
O	2.50175341	-1.37656955	3.19753193
C	-1.24396285	0.72269961	3.33984095
C	-3.57096194	1.97726718	4.30642619
C	-2.41922938	0.73628071	2.57627546

C	-1.25213668	1.33989502	4.60283475
C	-2.40812385	1.95910323	5.08131152
C	-3.57358255	1.36288767	3.05198494
H	-2.43672974	0.25212733	1.60446338
H	-0.35746066	1.32431010	5.21898875
H	-2.39658880	2.42768244	6.06131552
H	-4.47302147	1.36877209	2.44258023
H	-4.46781993	2.46452204	4.67769675

H in the Midpoint Total Energy = -1001.1895551

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.45000000
H	4.63173015	0.00000000	3.20871324
C	3.73754858	0.60855564	3.11958772
C	1.38349790	2.11974999	2.90228217
C	2.48689357	-0.02398662	3.10021488
C	3.79728683	1.99070783	3.02782038
C	2.61498392	2.75208706	2.91658457
C	1.28298139	0.70862896	3.00224389
H	4.76255838	2.48819696	3.04606839
H	2.67085814	3.83427823	2.84933083
H	0.47225470	2.70479733	2.82507993
H	2.45484066	-3.88686707	3.54478066
C	1.46143679	-3.45651299	3.46856990
C	-1.07320589	-2.26738131	3.30272489
C	0.31533013	-4.22998715	3.58467085
C	1.33354381	-2.07914825	3.26139294
C	0.07317415	-1.44963530	3.16266750
C	-0.95716988	-3.63250163	3.50816968
H	0.40456997	-5.29969925	3.74940582
H	-1.84948570	-4.24086989	3.61899076
H	-2.05565111	-1.80962626	3.26005514
C	-0.55156119	1.29144822	-0.53064326
H	-0.27057564	1.38323174	-1.59088398
H	-0.15190995	2.15789297	0.00658628
H	-1.64174368	1.31477614	-0.47200710
C	-0.60244598	-1.31060746	-0.40756781
H	-1.68931428	-1.30094947	-0.29460150
H	-0.17868217	-2.13675043	0.16961080
H	-0.36932019	-1.48617132	-1.46802218
O	1.34363037	-0.08293827	0.18919447
H	1.77780678	0.78594146	0.13082375
C	-0.00000057	-0.00000045	2.89999946
O	2.50175341	-1.37656955	3.19753193
C	-1.24396285	0.72269961	3.33984095
C	-3.57096194	1.97726718	4.30642619
C	-2.41922938	0.73628071	2.57627546

C	-1.25213668	1.33989502	4.60283475
C	-2.40812385	1.95910323	5.08131152
C	-3.57358255	1.36288767	3.05198494
H	-2.43672974	0.25212733	1.60446338
H	-0.35746066	1.32431010	5.21898875
H	-2.39658880	2.42768244	6.06131552
H	-4.47302147	1.36877209	2.44258023
H	-4.46781993	2.46452204	4.67769675

DAD = 3.1 Å

H in Donor WellTotal Energy =-1001.1867989

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.20000000
H	4.63612340	0.00000000	3.24195099
C	3.73942369	0.60911776	3.18909037
C	1.37875759	2.12181293	3.06822081
C	2.48888163	-0.02296717	3.21204650
C	3.79605595	1.99209412	3.10501220
C	2.61041899	2.75380592	3.04273925
C	1.28210255	0.71039840	3.16229382
H	4.76136142	2.48958697	3.09137773
H	2.66396161	3.83646241	2.98074823
H	0.46480647	2.70607329	3.02380410
H	2.46776952	-3.89039525	3.63800662
C	1.47313119	-3.45835115	3.59430647
C	-1.06531330	-2.26602937	3.51238094
C	0.32988069	-4.23122685	3.74091284
C	1.34035754	-2.07995728	3.39928921
C	0.07760584	-1.44857196	3.34291403
C	-0.94402850	-3.63233347	3.70554460
H	0.42276093	-5.30190813	3.89715118
H	-1.83300313	-4.24098786	3.83929812
H	-2.04774817	-1.80638438	3.50189636
C	-0.55743345	1.29067894	-0.51911838
H	-0.30750245	1.37691929	-1.58811374
H	-0.13967822	2.15809051	0.00233609
H	-1.64582402	1.31698869	-0.43000439
C	-0.60150877	-1.31098197	-0.39698189
H	-1.68785517	-1.30054579	-0.27903263
H	-0.17377579	-2.13328388	0.18215433
H	-0.37516279	-1.49193641	-1.45874517
O	1.34025212	-0.08071837	0.21265910
H	1.76658740	0.79428229	0.19259348
C	0.00000203	-0.00000130	3.09999644
O	2.50577379	-1.37707376	3.30070921
C	-1.24167004	0.71888865	3.55237723

C	-3.55919759	1.96842023	4.54075697
C	-2.41175144	0.76338988	2.78270723
C	-1.24648476	1.30519349	4.82984791
C	-2.39954166	1.92140923	5.31949422
C	-3.56232116	1.38782881	3.27019134
H	-2.42177941	0.30943731	1.79612043
H	-0.35288544	1.26814824	5.44690230
H	-2.38813122	2.36601457	6.31061346
H	-4.45873279	1.41984786	2.65714854
H	-4.45327706	2.45373037	4.92125521

H in Acceptor Well Total Energy = -1001.1868010

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.90000000
H	4.63612340	0.00000000	3.24195099
C	3.73942369	0.60911776	3.18909037
C	1.37875759	2.12181293	3.06822081
C	2.48888163	-0.02296717	3.21204650
C	3.79605595	1.99209412	3.10501220
C	2.61041899	2.75380592	3.04273925
C	1.28210255	0.71039840	3.16229382
H	4.76136142	2.48958697	3.09137773
H	2.66396161	3.83646241	2.98074823
H	0.46480647	2.70607329	3.02380410
H	2.46776952	-3.89039525	3.63800662
C	1.47313119	-3.45835115	3.59430647
C	-1.06531330	-2.26602937	3.51238094
C	0.32988069	-4.23122685	3.74091284
C	1.34035754	-2.07995728	3.39928921
C	0.07760584	-1.44857196	3.34291403
C	-0.94402850	-3.63233347	3.70554460
H	0.42276093	-5.30190813	3.89715118
H	-1.83300313	-4.24098786	3.83929812
H	-2.04774817	-1.80638438	3.50189636
C	-0.55743345	1.29067894	-0.51911838
H	-0.30750245	1.37691929	-1.58811374
H	-0.13967822	2.15809051	0.00233609
H	-1.64582402	1.31698869	-0.43000439
C	-0.60150877	-1.31098197	-0.39698189
H	-1.68785517	-1.30054579	-0.27903263
H	-0.17377579	-2.13328388	0.18215433
H	-0.37516279	-1.49193641	-1.45874517
O	1.34025212	-0.08071837	0.21265910
H	1.76658740	0.79428229	0.19259348
C	0.00000203	-0.00000130	3.09999644
O	2.50577379	-1.37707376	3.30070921
C	-1.24167004	0.71888865	3.55237723

C	-3.55919759	1.96842023	4.54075697
C	-2.41175144	0.76338988	2.78270723
C	-1.24648476	1.30519349	4.82984791
C	-2.39954166	1.92140923	5.31949422
C	-3.56232116	1.38782881	3.27019134
H	-2.42177941	0.30943731	1.79612043
H	-0.35288544	1.26814824	5.44690230
H	-2.38813122	2.36601457	6.31061346
H	-4.45873279	1.41984786	2.65714854
H	-4.45327706	2.45373037	4.92125521

H in the Midpoint Total Energy = -1001.18101627

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.55000000
H	4.63612340	0.00000000	3.24195099
C	3.73942369	0.60911776	3.18909037
C	1.37875759	2.12181293	3.06822081
C	2.48888163	-0.02296717	3.21204650
C	3.79605595	1.99209412	3.10501220
C	2.61041899	2.75380592	3.04273925
C	1.28210255	0.71039840	3.16229382
H	4.76136142	2.48958697	3.09137773
H	2.66396161	3.83646241	2.98074823
H	0.46480647	2.70607329	3.02380410
H	2.46776952	-3.89039525	3.63800662
C	1.47313119	-3.45835115	3.59430647
C	-1.06531330	-2.26602937	3.51238094
C	0.32988069	-4.23122685	3.74091284
C	1.34035754	-2.07995728	3.39928921
C	0.07760584	-1.44857196	3.34291403
C	-0.94402850	-3.63233347	3.70554460
H	0.42276093	-5.30190813	3.89715118
H	-1.83300313	-4.24098786	3.83929812
H	-2.04774817	-1.80638438	3.50189636
C	-0.55743345	1.29067894	-0.51911838
H	-0.30750245	1.37691929	-1.58811374
H	-0.13967822	2.15809051	0.00233609
H	-1.64582402	1.31698869	-0.43000439
C	-0.60150877	-1.31098197	-0.39698189
H	-1.68785517	-1.30054579	-0.27903263
H	-0.17377579	-2.13328388	0.18215433
H	-0.37516279	-1.49193641	-1.45874517
O	1.34025212	-0.08071837	0.21265910
H	1.76658740	0.79428229	0.19259348
C	0.00000203	-0.00000130	3.09999644
O	2.50577379	-1.37707376	3.30070921
C	-1.24167004	0.71888865	3.55237723

C	-3.55919759	1.96842023	4.54075697
C	-2.41175144	0.76338988	2.78270723
C	-1.24648476	1.30519349	4.82984791
C	-2.39954166	1.92140923	5.31949422
C	-3.56232116	1.38782881	3.27019134
H	-2.42177941	0.30943731	1.79612043
H	-0.35288544	1.26814824	5.44690230
H	-2.38813122	2.36601457	6.31061346
H	-4.45873279	1.41984786	2.65714854
H	-4.45327706	2.45373037	4.92125521

DAD = 3.5 Å

H in Donor WellTotal Energy = -1001.1787793

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.20000000
H	4.62703434	0.00000000	3.65629906
C	3.73090973	0.61034771	3.60787129
C	1.37058642	2.12660541	3.49947859
C	2.48027839	-0.01995421	3.61187103
C	3.78823989	1.99500890	3.55261906
C	2.60292372	2.75737191	3.49737213
C	1.27287873	0.71361031	3.56325848
H	4.75358915	2.49263524	3.55695154
H	2.65712126	3.84112529	3.45879665
H	0.45764833	2.71216135	3.45729288
H	2.45141651	-3.89601046	3.98764167
C	1.45831851	-3.46016151	3.94797273
C	-1.07889529	-2.26004529	3.87493231
C	0.31215574	-4.23099786	4.08220271
C	1.32920039	-2.07939756	3.77064579
C	0.06730482	-1.44342723	3.71873534
C	-0.96072180	-3.62832204	4.05090222
H	0.40141462	-5.30382364	4.22547124
H	-1.85106954	-4.23707393	4.17474107
H	-2.05955558	-1.79712204	3.86531207
C	-0.57329245	1.28972590	-0.49018116
H	-0.37936322	1.37035373	-1.57211033
H	-0.12651815	2.15678588	0.00576026
H	-1.65612613	1.31833117	-0.34679958
C	-0.59422535	-1.31062534	-0.38987971
H	-1.67734920	-1.31256287	-0.24540425
H	-0.14016789	-2.13257307	0.16762857
H	-0.39671474	-1.47498164	-1.46133945
O	1.33251707	-0.07163683	0.25938839
H	1.73827625	0.81237105	0.29643874
C	-0.00000045	0.00000087	3.49999534

O	2.49390331	-1.37720100	3.67375319
C	-1.26513713	0.72162965	3.87666494
C	-3.63751780	1.96327482	4.73644375
C	-2.39689149	0.74712637	3.04995297
C	-1.33614013	1.32428333	5.14467754
C	-2.51681672	1.93655093	5.57052546
C	-3.57385121	1.36731459	3.47409137
H	-2.34718969	0.28435427	2.06869559
H	-0.47379236	1.30206618	5.80559513
H	-2.55674053	2.39347381	6.55529456
H	-4.43975060	1.38543479	2.81794025
H	-4.55302274	2.44540392	5.06679215

H in Acceptor Well Total Energy = -1001.1788762

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	2.30000000
H	4.62703434	0.00000000	3.65629906
C	3.73090973	0.61034771	3.60787129
C	1.37058642	2.12660541	3.49947859
C	2.48027839	-0.01995421	3.61187103
C	3.78823989	1.99500890	3.55261906
C	2.60292372	2.75737191	3.49737213
C	1.27287873	0.71361031	3.56325848
H	4.75358915	2.49263524	3.55695154
H	2.65712126	3.84112529	3.45879665
H	0.45764833	2.71216135	3.45729288
H	2.45141651	-3.89601046	3.98764167
C	1.45831851	-3.46016151	3.94797273
C	-1.07889529	-2.26004529	3.87493231
C	0.31215574	-4.23099786	4.08220271
C	1.32920039	-2.07939756	3.77064579
C	0.06730482	-1.44342723	3.71873534
C	-0.96072180	-3.62832204	4.05090222
H	0.40141462	-5.30382364	4.22547124
H	-1.85106954	-4.23707393	4.17474107
H	-2.05955558	-1.79712204	3.86531207
C	-0.57329245	1.28972590	-0.49018116
H	-0.37936322	1.37035373	-1.57211033
H	-0.12651815	2.15678588	0.00576026
H	-1.65612613	1.31833117	-0.34679958
C	-0.59422535	-1.31062534	-0.38987971
H	-1.67734920	-1.31256287	-0.24540425
H	-0.14016789	-2.13257307	0.16762857
H	-0.39671474	-1.47498164	-1.46133945
O	1.33251707	-0.07163683	0.25938839
H	1.73827625	0.81237105	0.29643874
C	-0.00000045	0.00000087	3.49999534

O	2.49390331	-1.37720100	3.67375319
C	-1.26513713	0.72162965	3.87666494
C	-3.63751780	1.96327482	4.73644375
C	-2.39689149	0.74712637	3.04995297
C	-1.33614013	1.32428333	5.14467754
C	-2.51681672	1.93655093	5.57052546
C	-3.57385121	1.36731459	3.47409137
H	-2.34718969	0.28435427	2.06869559
H	-0.47379236	1.30206618	5.80559513
H	-2.55674053	2.39347381	6.55529456
H	-4.43975060	1.38543479	2.81794025
H	-4.55302274	2.44540392	5.06679215

H in the Midpoint Total Energy = -1001.1594064

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.75000000
H	4.62703434	0.00000000	3.65629906
C	3.73090973	0.61034771	3.60787129
C	1.37058642	2.12660541	3.49947859
C	2.48027839	-0.01995421	3.61187103
C	3.78823989	1.99500890	3.55261906
C	2.60292372	2.75737191	3.49737213
C	1.27287873	0.71361031	3.56325848
H	4.75358915	2.49263524	3.55695154
H	2.65712126	3.84112529	3.45879665
H	0.45764833	2.71216135	3.45729288
H	2.45141651	-3.89601046	3.98764167
C	1.45831851	-3.46016151	3.94797273
C	-1.07889529	-2.26004529	3.87493231
C	0.31215574	-4.23099786	4.08220271
C	1.32920039	-2.07939756	3.77064579
C	0.06730482	-1.44342723	3.71873534
C	-0.96072180	-3.62832204	4.05090222
H	0.40141462	-5.30382364	4.22547124
H	-1.85106954	-4.23707393	4.17474107
H	-2.05955558	-1.79712204	3.86531207
C	-0.57329245	1.28972590	-0.49018116
H	-0.37936322	1.37035373	-1.57211033
H	-0.12651815	2.15678588	0.00576026
H	-1.65612613	1.31833117	-0.34679958
C	-0.59422535	-1.31062534	-0.38987971
H	-1.67734920	-1.31256287	-0.24540425
H	-0.14016789	-2.13257307	0.16762857
H	-0.39671474	-1.47498164	-1.46133945
O	1.33251707	-0.07163683	0.25938839
H	1.73827625	0.81237105	0.29643874
C	-0.00000045	0.00000087	3.49999534

O	2.49390331	-1.37720100	3.67375319
C	-1.26513713	0.72162965	3.87666494
C	-3.63751780	1.96327482	4.73644375
C	-2.39689149	0.74712637	3.04995297
C	-1.33614013	1.32428333	5.14467754
C	-2.51681672	1.93655093	5.57052546
C	-3.57385121	1.36731459	3.47409137
H	-2.34718969	0.28435427	2.06869559
H	-0.47379236	1.30206618	5.80559513
H	-2.55674053	2.39347381	6.55529456
H	-4.43975060	1.38543479	2.81794025
H	-4.55302274	2.44540392	5.06679215

Table S7. The atom coordinates and absolute energies of the TRS at different DADs for the reaction of Xn^+ (for Figure 1 in the paper) (The geometry of the Xn^+ reaction from the previous paper[1] is further refined to obtain the symmetrical double potential wells (fitted to the 6th-order polynomial) so that the small barrier difference at the bottom of the double potential wells from that of the reaction of $PhXn^+$ can be clearly recognized. Note that the 2° KIEs resulted from the refined geometries are the same as the ones in Table 1 in the paper within the calculation error.)

DAD = 2.9 Å

H in Donor WellTotal Energy = -770.1374367

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.28500000
O	2.78798392	0.00000000	3.39181800
C	2.11874512	-1.18422272	3.32906828
C	-0.00000006	-0.00000206	2.89999429
C	2.10837230	1.18422627	3.37809487
C	0.70899350	1.23328920	3.19144167
C	0.71943540	-1.23871339	3.13981291
C	2.85878174	2.34490233	3.58693808
H	3.93242731	2.26705507	3.72303593
C	2.20281234	3.56862633	3.62482218
H	2.77675636	4.47520799	3.79055065
C	0.06976609	2.49359953	3.24870146
H	-1.00929358	2.54254321	3.12403749
C	0.80399155	3.64668901	3.46770747
H	0.30561021	4.60957465	3.51800389
C	2.87729936	-2.34958989	3.49234394
H	3.94966317	-2.26843589	3.63754729
C	2.23153763	-3.57881682	3.47774850
H	2.81183951	-4.48664850	3.61182801
C	0.09040057	-2.50630251	3.14107909
H	-0.98916269	-2.55709888	3.01998792
C	0.83328804	-3.66201634	3.31183085

H	0.34238744	-4.63006113	3.32420361
O	1.32774598	-0.25266702	0.09450990
H	1.52332321	-1.20411449	0.03141085
C	-0.91011627	-1.10532695	-0.45162926
H	-0.81876275	-1.22542196	-1.54150697
H	-1.95341977	-0.86378890	-0.23027209
H	-0.66025436	-2.06072550	0.02272948
H	-1.07252067	-0.00335730	3.08910934
C	-0.29822227	1.41960767	-0.37598784
H	-1.33757038	1.67370440	-0.15198798
H	-0.14173797	1.53664065	-1.45854133
H	0.37223310	2.11245919	0.13901443

H in Acceptor Well Total Energy = -770.1374947

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.61500000
O	2.78798392	0.00000000	3.39181800
C	2.11874512	-1.18422272	3.32906828
C	-0.00000006	-0.00000206	2.89999429
C	2.10837230	1.18422627	3.37809487
C	0.70899350	1.23328920	3.19144167
C	0.71943540	-1.23871339	3.13981291
C	2.85878174	2.34490233	3.58693808
H	3.93242731	2.26705507	3.72303593
C	2.20281234	3.56862633	3.62482218
H	2.77675636	4.47520799	3.79055065
C	0.06976609	2.49359953	3.24870146
H	-1.00929358	2.54254321	3.12403749
C	0.80399155	3.64668901	3.46770747
H	0.30561021	4.60957465	3.51800389
C	2.87729936	-2.34958989	3.49234394
H	3.94966317	-2.26843589	3.63754729
C	2.23153763	-3.57881682	3.47774850
H	2.81183951	-4.48664850	3.61182801
C	0.09040057	-2.50630251	3.14107909
H	-0.98916269	-2.55709888	3.01998792
C	0.83328804	-3.66201634	3.31183085
H	0.34238744	-4.63006113	3.32420361
O	1.32774598	-0.25266702	0.09450990
H	1.52332321	-1.20411449	0.03141085
C	-0.91011627	-1.10532695	-0.45162926
H	-0.81876275	-1.22542196	-1.54150697
H	-1.95341977	-0.86378890	-0.23027209
H	-0.66025436	-2.06072550	0.02272948
H	-1.07252067	-0.00335730	3.08910934
C	-0.29822227	1.41960767	-0.37598784
H	-1.33757038	1.67370440	-0.15198798

H	-0.14173797	1.53664065	-1.45854133
H	0.37223310	2.11245919	0.13901443

H in the Midpoint Total Energy =-770.1368891

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.45000000
O	2.78798392	0.00000000	3.39181800
C	2.11874512	-1.18422272	3.32906828
C	-0.00000006	-0.00000206	2.89999429
C	2.10837230	1.18422627	3.37809487
C	0.70899350	1.23328920	3.19144167
C	0.71943540	-1.23871339	3.13981291
C	2.85878174	2.34490233	3.58693808
H	3.93242731	2.26705507	3.72303593
C	2.20281234	3.56862633	3.62482218
H	2.77675636	4.47520799	3.79055065
C	0.06976609	2.49359953	3.24870146
H	-1.00929358	2.54254321	3.12403749
C	0.80399155	3.64668901	3.46770747
H	0.30561021	4.60957465	3.51800389
C	2.87729936	-2.34958989	3.49234394
H	3.94966317	-2.26843589	3.63754729
C	2.23153763	-3.57881682	3.47774850
H	2.81183951	-4.48664850	3.61182801
C	0.09040057	-2.50630251	3.14107909
H	-0.98916269	-2.55709888	3.01998792
C	0.83328804	-3.66201634	3.31183085
H	0.34238744	-4.63006113	3.32420361
O	1.32774598	-0.25266702	0.09450990
H	1.52332321	-1.20411449	0.03141085
C	-0.91011627	-1.10532695	-0.45162926
H	-0.81876275	-1.22542196	-1.54150697
H	-1.95341977	-0.86378890	-0.23027209
H	-0.66025436	-2.06072550	0.02272948
H	-1.07252067	-0.00335730	3.08910934
C	-0.29822227	1.41960767	-0.37598784
H	-1.33757038	1.67370440	-0.15198798
H	-0.14173797	1.53664065	-1.45854133
H	0.37223310	2.11245919	0.13901443

DAD = 3.1 Å

H in Donor Well Total Energy =-770.134196286

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.20000000

O	2.78504036	0.00000000	3.60324882
C	0.00000004	0.00000000	3.09999879
C	2.11651323	-1.18436970	3.53940237
C	2.10582215	1.18338450	3.58859257
C	0.70784269	1.23226785	3.38696183
C	0.71902514	-1.23818575	3.33439477
C	2.85441711	2.34155326	3.81616964
H	3.92577354	2.26102806	3.96880122
C	2.19820288	3.56483422	3.85766651
H	2.76993756	4.46992999	4.04037465
C	0.06908569	2.49314965	3.44411961
H	-1.00818984	2.54361696	3.30614590
C	0.80117404	3.64387045	3.68100076
H	0.30275744	4.60669340	3.73379876
C	2.87394711	-2.34749004	3.71971747
H	3.94375929	-2.26402711	3.88220302
C	2.22919669	-3.57707642	3.70480714
H	2.80800021	-4.48403629	3.85316854
C	0.09180234	-2.50667414	3.33156196
H	-0.98558564	-2.55927787	3.19334203
C	0.83337264	-3.66093344	3.51715267
H	0.34332467	-4.62951821	3.52639905
O	1.32776591	-0.25256579	0.09451118
H	1.52007464	-1.20612488	0.05280954
C	-0.90762930	-1.10546330	-0.45091490
H	-0.80774541	-1.22669303	-1.54044720
H	-1.95230925	-0.86427968	-0.23791701
H	-0.65930980	-2.06039863	0.02467847
H	-1.07252127	-0.00343806	3.28911421
C	-0.29536172	1.42168333	-0.36431068
H	-1.33648272	1.67431309	-0.14880433
H	-0.12843342	1.54784181	-1.44471611
H	0.37238863	2.10943434	0.16073030

H in Acceptor Well Total Energy = -770.133336821

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.90000000
O	2.78504036	0.00000000	3.60324882
C	0.00000004	0.00000000	3.09999879
C	2.11651323	-1.18436970	3.53940237
C	2.10582215	1.18338450	3.58859257
C	0.70784269	1.23226785	3.38696183
C	0.71902514	-1.23818575	3.33439477
C	2.85441711	2.34155326	3.81616964
H	3.92577354	2.26102806	3.96880122
C	2.19820288	3.56483422	3.85766651

H	2.76993756	4.46992999	4.04037465
C	0.06908569	2.49314965	3.44411961
H	-1.00818984	2.54361696	3.30614590
C	0.80117404	3.64387045	3.68100076
H	0.30275744	4.60669340	3.73379876
C	2.87394711	-2.34749004	3.71971747
H	3.94375929	-2.26402711	3.88220302
C	2.22919669	-3.57707642	3.70480714
H	2.80800021	-4.48403629	3.85316854
C	0.09180234	-2.50667414	3.33156196
H	-0.98558564	-2.55927787	3.19334203
C	0.83337264	-3.66093344	3.51715267
H	0.34332467	-4.62951821	3.52639905
O	1.32776591	-0.25256579	0.09451118
H	1.52007464	-1.20612488	0.05280954
C	-0.90762930	-1.10546330	-0.45091490
H	-0.80774541	-1.22669303	-1.54044720
H	-1.95230925	-0.86427968	-0.23791701
H	-0.65930980	-2.06039863	0.02467847
H	-1.07252127	-0.00343806	3.28911421
C	-0.29536172	1.42168333	-0.36431068
H	-1.33648272	1.67431309	-0.14880433
H	-0.12843342	1.54784181	-1.44471611
H	0.37238863	2.10943434	0.16073030

H in the Midpoint Total Energy =-770.128696

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.55000000
O	2.78504036	0.00000000	3.60324882
C	0.00000004	0.00000000	3.09999879
C	2.11651323	-1.18436970	3.53940237
C	2.10582215	1.18338450	3.58859257
C	0.70784269	1.23226785	3.38696183
C	0.71902514	-1.23818575	3.33439477
C	2.85441711	2.34155326	3.81616964
H	3.92577354	2.26102806	3.96880122
C	2.19820288	3.56483422	3.85766651
H	2.76993756	4.46992999	4.04037465
C	0.06908569	2.49314965	3.44411961
H	-1.00818984	2.54361696	3.30614590
C	0.80117404	3.64387045	3.68100076
H	0.30275744	4.60669340	3.73379876
C	2.87394711	-2.34749004	3.71971747
H	3.94375929	-2.26402711	3.88220302
C	2.22919669	-3.57707642	3.70480714
H	2.80800021	-4.48403629	3.85316854

C	0.09180234	-2.50667414	3.33156196
H	-0.98558564	-2.55927787	3.19334203
C	0.83337264	-3.66093344	3.51715267
H	0.34332467	-4.62951821	3.52639905
O	1.32776591	-0.25256579	0.09451118
H	1.52007464	-1.20612488	0.05280954
C	-0.90762930	-1.10546330	-0.45091490
H	-0.80774541	-1.22669303	-1.54044720
H	-1.95230925	-0.86427968	-0.23791701
H	-0.65930980	-2.06039863	0.02467847
H	-1.07252127	-0.00343806	3.28911421
C	-0.29536172	1.42168333	-0.36431068
H	-1.33648272	1.67431309	-0.14880433
H	-0.12843342	1.54784181	-1.44471611
H	0.37238863	2.10943434	0.16073030

DAD = 3.5 Å

H in Donor WellTotal Energy = -770.1242507

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.20000000
O	2.80730361	0.00000000	3.74372989
C	2.14097076	-1.18767360	3.71731740
C	0.00000266	-0.00000097	3.50000100
C	2.12762902	1.17931081	3.84865507
C	0.71737574	1.22505408	3.76489671
C	0.72982145	-1.23914886	3.63901294
C	2.88750294	2.33246559	4.06123498
H	3.96820261	2.25504375	4.12242157
C	2.22967446	3.54755445	4.20879644
H	2.80961505	4.44899406	4.38352820
C	0.07860866	2.47617616	3.92664048
H	-1.00614578	2.52340307	3.87277464
C	0.82252901	3.62214579	4.14942219
H	0.32587346	4.57834071	4.28090690
C	2.91308399	-2.35100332	3.79671761
H	3.99344114	-2.26919907	3.85796835
C	2.26916982	-3.58135818	3.81584587
H	2.85921253	-4.49024276	3.88851571
C	0.10460114	-2.50864879	3.66912572
H	-0.98077061	-2.56046641	3.62744811
C	0.86142112	-3.66418781	3.75979883
H	0.37516722	-4.63413286	3.79561764
O	1.05979679	-0.84147768	0.14700495
H	0.77540021	-1.77247438	0.17408356
C	-1.31388714	-0.55900786	-0.44397468

H	-1.28886533	-0.68633084	-1.53804393
H	-2.12899981	0.13004189	-0.20934462
H	-1.52812522	-1.53119566	0.01038231
H	-1.05557439	-0.01355063	3.76320966
C	0.40022640	1.39352286	-0.34923542
H	-0.39142011	2.10343536	-0.09826445
H	0.56817733	1.44410143	-1.43681159
H	1.32980599	1.67561442	0.14961378

H in Acceptor Well Total Energy = -770.1241509

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	2.30000040
O	2.80730361	0.00000000	3.74372989
C	2.14097076	-1.18767360	3.71731740
C	0.00000266	-0.00000097	3.50000100
C	2.12762902	1.17931081	3.84865507
C	0.71737574	1.22505408	3.76489671
C	0.72982145	-1.23914886	3.63901294
C	2.88750294	2.33246559	4.06123498
H	3.96820261	2.25504375	4.12242157
C	2.22967446	3.54755445	4.20879644
H	2.80961505	4.44899406	4.38352820
C	0.07860866	2.47617616	3.92664048
H	-1.00614578	2.52340307	3.87277464
C	0.82252901	3.62214579	4.14942219
H	0.32587346	4.57834071	4.28090690
C	2.91308399	-2.35100332	3.79671761
H	3.99344114	-2.26919907	3.85796835
C	2.26916982	-3.58135818	3.81584587
H	2.85921253	-4.49024276	3.88851571
C	0.10460114	-2.50864879	3.66912572
H	-0.98077061	-2.56046641	3.62744811
C	0.86142112	-3.66418781	3.75979883
H	0.37516722	-4.63413286	3.79561764
O	1.05979679	-0.84147768	0.14700495
H	0.77540021	-1.77247438	0.17408356
C	-1.31388714	-0.55900786	-0.44397468
H	-1.28886533	-0.68633084	-1.53804393
H	-2.12899981	0.13004189	-0.20934462
H	-1.52812522	-1.53119566	0.01038231
H	-1.05557439	-0.01355063	3.76320966
C	0.40022640	1.39352286	-0.34923542
H	-0.39142011	2.10343536	-0.09826445
H	0.56817733	1.44410143	-1.43681159
H	1.32980599	1.67561442	0.14961378

H in the Midpoint Total Energy =-770.10496395

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.75000000
O	2.80730361	0.00000000	3.74372989
C	2.14097076	-1.18767360	3.71731740
C	0.00000266	-0.00000097	3.50000100
C	2.12762902	1.17931081	3.84865507
C	0.71737574	1.22505408	3.76489671
C	0.72982145	-1.23914886	3.63901294
C	2.88750294	2.33246559	4.06123498
H	3.96820261	2.25504375	4.12242157
C	2.22967446	3.54755445	4.20879644
H	2.80961505	4.44899406	4.38352820
C	0.07860866	2.47617616	3.92664048
H	-1.00614578	2.52340307	3.87277464
C	0.82252901	3.62214579	4.14942219
H	0.32587346	4.57834071	4.28090690
C	2.91308399	-2.35100332	3.79671761
H	3.99344114	-2.26919907	3.85796835
C	2.26916982	-3.58135818	3.81584587
H	2.85921253	-4.49024276	3.88851571
C	0.10460114	-2.50864879	3.66912572
H	-0.98077061	-2.56046641	3.62744811
C	0.86142112	-3.66418781	3.75979883
H	0.37516722	-4.63413286	3.79561764
O	1.05979679	-0.84147768	0.14700495
H	0.77540021	-1.77247438	0.17408356
C	-1.31388714	-0.55900786	-0.44397468
H	-1.28886533	-0.68633084	-1.53804393
H	-2.12899981	0.13004189	-0.20934462
H	-1.52812522	-1.53119566	0.01038231
H	-1.05557439	-0.01355063	3.76320966
C	0.40022640	1.39352286	-0.34923542
H	-0.39142011	2.10343536	-0.09826445
H	0.56817733	1.44410143	-1.43681159
H	1.32980599	1.67561442	0.14961378

Table S8. The atom coordinates and absolute energies of the classical TS at DAD = 2.767 Å for the reaction of 2-propanol with $PhXn^+$

H in Acceptor Well Total Energy = -1001.20561267

H	-2.42035	-3.9587	0.506
C	-2.47476	-2.88415	0.36239

C	-2.53802	-0.11652	-0.04196
C	-1.28902	-2.17393	0.12568
C	-3.68291	-2.20123	0.39796
C	-3.71792	-0.80928	0.19489
C	-1.29114	-0.78152	-0.08487
H	-4.60408	-2.74913	0.57406
H	-4.66559	-0.27953	0.20984
H	-2.56683	0.95387	-0.22531
H	1.97265	-4.26496	-0.19943
C	2.12577	-3.20644	-0.38467
C	2.42991	-0.47182	-0.88794
C	3.36079	-2.70092	-0.76897
C	1.04212	-2.33252	-0.24558
C	1.16583	-0.95048	-0.4803
C	3.51301	-1.32844	-1.02903
H	4.20506	-3.37459	-0.88246
H	4.47405	-0.93778	-1.34935
H	2.54823	0.58425	-1.10939
C	0.20342	0.5527	2.42647
H	0.19061	0.44924	0.83577
C	-0.64806	1.77537	2.59862
H	-0.74534	1.96948	3.67817
H	-1.65368	1.63329	2.18834
H	-0.1936	2.65291	2.13722
C	1.68492	0.58529	2.61882
H	2.12452	1.49276	2.20048
H	2.15818	-0.29811	2.17959
H	1.88889	0.56855	3.70012
O	-0.32825	-0.6258	2.72522
H	-1.30469	-0.61143	2.71039
C	-0.00576	-0.04162	-0.26442
O	-0.14824	-2.91558	0.09803
C	-0.06165	1.17377	-1.18391
C	-0.09128	3.34581	-2.97281
C	0.52794	2.39544	-0.83538
C	-0.65929	1.04853	-2.4485
C	-0.67221	2.12631	-3.33487
C	0.51145	3.47783	-1.7206
H	1.01821	2.50955	0.12847
H	-1.1101	0.1049	-2.74315
H	-1.13736	2.01152	-4.31009
H	0.97101	4.41873	-1.43068
H	-0.10645	4.18442	-3.66289

Table S9. The atom coordinates and absolute energies of the classical TS at DAD = 2.778 Å for the reaction of 2-propanol with Xn^+

H in Acceptor Well Total Energy = -770.149558678

H	-0.97355	2.91312	-2.8347
C	-0.8164	2.85669	-1.7623
C	-0.45695	2.6493	1.01087
C	-0.81724	1.60624	-1.13725
C	-0.63629	3.99739	-0.98801
C	-0.46443	3.89843	0.40384
C	-0.62594	1.47639	0.24943
H	-0.64352	4.97302	-1.46487
H	-0.34305	4.79595	1.0023
H	-0.33031	2.56631	2.08814
C	-0.57905	0.12124	0.84811
H	-0.93038	0.08357	1.88597
C	-1.1397	-0.94569	-0.01254
C	-2.05594	-2.95816	-1.74757
C	-1.29785	-0.70265	-1.39013
C	-1.47582	-2.22336	0.48224
C	-1.92964	-3.22208	-0.37107
C	-1.74679	-1.7038	-2.25954
H	-1.40215	-2.41164	1.55169
H	-2.20094	-4.19627	0.02391
H	-1.85891	-1.47478	-3.31452
H	-2.4148	-3.73447	-2.41687
O	-1.04182	0.5184	-1.94344
C	2.03663	-0.80732	0.73644
H	0.57217	-0.15092	1.00276
O	1.78802	-1.44049	-0.39657
H	1.38993	-2.32382	-0.26533
C	2.77368	0.47772	0.54899
H	3.82051	0.23896	0.30674
H	2.7608	1.08038	1.4594
H	2.36287	1.05017	-0.28802
C	2.13185	-1.59608	2.00769
H	3.11611	-2.0898	2.02953
H	1.36304	-2.37415	2.06972
H	2.06587	-0.94779	2.88498

References

(1) Kashefolgheta, S.; Razzaghi, M.; Hammann, B.; Eilers, J.; Roston, D.; Lu, Y.: Computational Replication of the Abnormal Secondary Kinetic Isotope Effects in a Hydride Transfer Reaction in Solution with a Motion Assisted H-Tunneling Model. *J. Org. Chem.* **2014**, *79*, 1989-1994.