Supporting Information for

Electron Density Deformations provide new

Insights into the Spectral Shift of Rhodopsins

Erix Wiliam Hernández-Rodríguez,^{1,2,3} Ana Lilian Montero-Alejo,³ Rafael López,² Elsa Sánchez-García,⁴ Luis Alberto Montero-Cabrera,³ and José Manuel García de la Vega²

1) Departamento de Bioquímica, Instituto de Ciencias Básicas y Preclínicas "Victoria de Girón", Universidad de Ciencias Médicas de La Habana, 11600 -Havana, Cuba.

2)Departamento de Química Física Aplicada, Facultad de Ciencias, Universidad Autónoma de Madrid, 28049- Madrid, Spain.

3)Laboratorio de Química Computacional y Teórica.Departamento de Química Física, Universidad de La Habana, 10400 - Havana, Cuba.

4)Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany.

Keywords: rhodopsin, mutations, *Retinitis Pigmentosa*, electronic structure, electron density deformations

Figure S1. Overlay of the QM regions of bWT (a), hWT (b), hM207R (c) and hS186W (d) from four snapshots of each system. **Rho**₁ model: protein in explicit water environment, the QM region includes 11-*cis*-retinal, part of Lys296, part of Glu113 and two water molecules (W6 and W8).



Tables S1a – S1d contain the corresponding Cartesian coordinates for each QM region (bWT, hWT, hM207R and hS186W) of **Rho**₁ model.

Figure S2. QM regions of hWT (a), hM207R (b) and hS186W (c) from one snapshot of each system. **Rho**₂ model: the QM region only contains 11-*cis*-retinal and part of Lys296. All MM point charges are set to zero except those of Glu113.



Table S2 contains the corresponding Cartesian coordinates for each QM region (hWT, hM207R and hS186W) of **Rho**₂ model.

Figure S3. QM region of hWT from **Ret**_{gas} model: the QM region only contains 11*cis*-retinal and part of Lys296. All MM point charges are set to zero, for hWT. SBR is deprotonated.



Table S3 contains the corresponding Cartesian coordinates for the QM region (hWT) of Ret_{gas} model.

Figure S4. Overlay of the QM regions of bWT (a), hWT (b) and hS186W (c) from three snapshots of each system. **Rho₃** model: protein in a solvated lipid bilayer of palmitoyl-oleoyl-phosphatidyl-choline, the same QM region as above (**Rho₁**). The snapshots are obtained from completely unconstrained simulations used previously¹ for identifying large structural deviations of the rhodopsins compared with the crystal structure.



Tables S4a – S4c contain the corresponding Cartesian coordinates for each QM region (bWT, hWT and hS186W) of **Rho₃** model.

1. Hernández-Rodríguez, E. W.; Sánchez-García, E.; Crespo-Otero, R.; Montero-Alejo, A. L.; Montero, L. A.; Thiel, W., *J. Phys. Chem. B* 2012, *116* (3), 1060-76.

Figure S5. QM regions of hWT (a), hM207R (b) and hS186W (c) from one snapshot of each system. **Rho₄** model: using the **Rho₁** model but Glu113 (counterion) and water molecules were excluded from the QM region.



Table S5 contains the corresponding Cartesian coordinates for each QM region (hWT, hM207R and hS186W) of **Rho**₄ model.

Figure S6. QM regions of hWT (a), hM207R (b) and hS186W (c) from one snapshot of each system. **Rho₅** model: using the **Rho₁** model but the QM region only contains 11-*cis*-retinal and part of Lys296. All MM point charges were retained except those of Glu113.



Table S6 contains the corresponding Cartesian coordinates for each QM region (hWT, hM207R and hS186W) of **Rho**₅ model.

Figure S7. QM region of hS186W for Rho_6 model: using the Ret_{gas} model but applied to hS186W.



Table S7 contains the corresponding Cartesian coordinates for the QM region (hS186W) of \mathbf{Rho}_6 model.

Table S1a. Cartesian coordinates (in Å) of the QM region of bWT snapshots. Rho_1

mod	del

A 4	T		bWT1			bWT2			bWT3			bWT4	
Atom	Type	х	У	Z	х	У	Z	х	У	z	х	У	Z
1	С	-7,70504104	-2,84672947	-1,18771056	-7,85601330	-2,75760149	-1,14122924	-7,82442221	-2,77902486	-1,13996968	-7,67855001	-2,90844536	-1,16560264
2	Η	-8,12070358	-2,24597366	-1,99722786	-8,28188081	-2,14509666	-1,93505533	-8,25848377	-2,17240612	-1,93516993	-8,12308631	-2,32468459	-1,97222091
3	Н	-8,51631120	-2,98777689	-0,46001314	-8,64292024	-2,87521909	-0,38282782	-8,61251753	-2,92887235	-0,38833301	-8,46578779	-3,05085804	-0,41191540
4	С	-6,63091886	-2,03194037	-0,43698911	-6,73667292	-1,97505406	-0,43179493	-6,72053820	-1,98423955	-0,41900521	-6,59197126	-2,07667914	-0,46170349
5	0	-5,/3////20	-2,60/23858	0,20/3292/	-5,83458246	-2,56337853	0,18519484	-5,83316622	-2,56802178	0,2236/551	-5,6/5/0445	-2,62656233	0,17158378
7	C	-6,78428723	4 97972906	-0,49118694	-6,86207613	-0,08983981	-0,48086241	-6,84314201	-0,70182022	-0,48540727	-6,75790997	-0,79926389	-0,53251946
8	н	-4.81102312	5.11651820	0.90814474	-4.83059791	5.15063947	0.98031530	-4.80158285	5.06296551	0.91178726	-4.86762774	5.10244535	0.90158281
9	н	-5,73871311	5,78792416	-0,41946772	-5,70204007	5,76491299	-0,41295820	-5,76889172	5,75837998	-0,37331576	-5,78485154	5,77946499	-0,42856994
10	С	-6,30455837	3,77149993	0,09329260	-6,24602205	3,74973456	0,11786956	-6,32412015	3,73486210	0,12578203	-6,37531762	3,77279069	0,08534236
11	Н	-7,19844807	4,23541159	0,51766905	-7,16014786	4,19438775	0,51825282	-7,20665064	4,19738071	0,57504997	-7,26005446	4,24489654	0,51980867
12	Η	-6,62050137	3,36560901	-0,87314351	-6,52489158	3,33975773	-0,85776406	-6,66481102	3,33222616	-0,83313465	-6,70249426	3,37876572	-0,88249282
13	С	-5,98232017	2,61398778	1,05697643	-5,90884179	2,59595049	1,08537469	-5,97394869	2,57649327	1,07983863	-6,06049569	2,60454627	1,03975816
14	H	-5,40528090	2,98337242	1,90485014	-5,29718306	2,96552237	1,90930209	-5,38933230	2,94862730	1,92089101	-5,50854741	2,97043291	1,90622296
15	п N	-6,91601056	2,21300641	1,44635204	-6,8341/388	2,21613591	1,51218563	-6,89/61515	2,16631793	1,4834/543	-6,99676031	2,18545969	1,40418123
17	н	-5 80894424	0 69774764	0,45020087	-5 79596575	0.68726068	0.05811576	-5 79741463	0.67832262	0,49932937	-5 83211199	0 70419378	0.01746661
18	č	6.97277546	-0.03734237	0.74586455	7.01709718	-0.10069244	0.71160321	7.01922717	-0.05898105	0.74091083	6.98798216	-0.07363921	0.74147518
19	С	7,74084920	1,30025472	0,76406138	7,78232992	1,23398717	0,81159599	7,78986270	1,27564014	0,78459782	7,82365332	1,22355209	0,75403647
20	Н	7,09898561	2,06345274	1,22019526	7,14615848	1,96048480	1,33100072	7,14931211	2,02811425	1,25881703	7,22686346	2,01805507	1,21766890
21	Н	8,61916479	1,19975120	1,40885197	8,67109851	1,09218512	1,43399686	8,67143231	1,16008625	1,42345890	8,70240061	1,07692141	1,38863388
22	С	8,14589628	1,76894195	-0,62500287	8,16496857	1,80272075	-0,54760788	8,18813277	1,77944313	-0,59540250	8,23246036	1,67499684	-0,64043109
23	Н	8,69606477	2,71140449	-0,56004027	8,71438156	2,74022330	-0,42260991	8,74212838	2,71750077	-0,50858148	8,83768901	2,58409429	-0,58002172
24	H	8,82683384	1,04605776	-1,08214579	8,84032521	1,11750312	-1,06579639	8,86045194	1,06605285	-1,07987893	8,86135556	0,91758570	-1,11383298
25	С	6,91093946	1,94389942	-1,50256305	6,91808494	2,03382303	-1,39405361	6,94602354	1,98561022	-1,45375045	6,99281413	1,92583110	-1,49189615
20	п	6,44223960 7 20122112	2,91980059	-1,3089/955	5,45374683	2,99568809	-1,13553296	0,4/8/8628	2,952/101/	-1,21/96628	0,57808612	2,92010706	-1,2/63/30/
28	C	5 8/309829	0 89013708	-2,53770003	5 85042597	0.97160231	-2,44943670	5 88369233	0.921/29/8	-2,31082178	5 88012837	0.91958400	-2,33309112
20	C	5 82855248	0,02096110	-0.29069315	5,85138357	0.03313887	-0 29543765	5,88509255	0,92142948	-0.28703729	5,88012857	0.04054679	-0 28740930
30	č	4.76333198	-0.97635911	-0.11647769	4,78730606	-0.96902421	-0.16354556	4.80614268	-0.97909454	-0.14033550	4,74667354	-0.92630203	-0.12528709
31	Н	5,08353878	-1,98248306	0,14323060	5,11007387	-1,98721405	0,04129477	5,12850096	-1,99617512	0,06902643	5,04551733	-1,95408841	0,07001453
32	С	3,44161270	-0,71696775	-0,20645848	3,46425489	-0,70894876	-0,22343414	3,48376005	-0,71338904	-0,20296965	3,42878042	-0,63537948	-0,16270457
33	Н	3,15309380	0,30996415	-0,39776423	3,16658706	0,32374114	-0,36012215	3,19764199	0,32203609	-0,33977040	3,14660613	0,40506183	-0,28373653
34	С	2,34093313	-1,65121802	-0,09362574	2,37019991	-1,65573388	-0,14196660	2,38158140	-1,65267579	-0,13185740	2,32805503	-1,57610213	-0,08258685
35	С	1,07245436	-1,14040927	-0,16089626	1,09759373	-1,15160764	-0,19208176	1,11071123	-1,13894519	-0,14776863	1,05731872	-1,06855749	-0,09411780
36	Н	1,00564643	-0,06489488	-0,24548745	1,02335844	-0,07320394	-0,23612444	1,04298269	-0,05999240	-0,15976406	0,98397876	0,00919852	-0,10513682
37	С	-0,16062297	-1,86469789	-0,21451156	-0,12578773	-1,88795815	-0,28167548	-0,12302410	-1,85763099	-0,23453947	-0,17081516	-1,79836580	-0,17278997
38	н	-0,07752203	-2,91520688	-0,47906832	-0,02981681	-2,92343144	-0,59520036	-0,04135048	-2,89703047	-0,53852519	-0,08087563	-2,84284638	-0,45532028
39 40	ч	-1,44256087	-1,40500663	-0,08322010	-1,41392342	-1,44553145	-0,14063885	-1,40770229	-1,40362356	-0,09649784	-1,45/8384/	-1,35289405	-0,04237835
40	C	-2,22307003	-2,12558000	0 37572693	-1 93341201	-0.20099221	0 36643512	-2,18323302	-2,11758195	0 38738812	-2,22930093	-2,07824000	0.41338763
42	c	-3.30950903	0.07576438	0.25018608	-3.28861955	0.02091103	0.22991853	-3.28780622	0.05961625	0.24889233	-3.34091054	0.10648939	0.27284445
43	Н	-3,92340204	-0,70597601	-0,18705814	-3,90288814	-0,73960563	-0,24254278	-3,89318973	-0,71402940	-0,21138954	-3,94187372	-0,68102962	-0,17207827
44	С	-3,97980097	1,24088220	0,68760291	-3,94695302	1,17947031	0,69417251	-3,96773950	1,21370562	0,70220212	-4,03125760	1,26215152	0,70324809
45	Η	-3,45050424	2,02214424	1,22415092	-3,40440069	1,93903090	1,24859641	-3,44527536	1,98733139	1,25773302	-3,52560151	2,04511665	1,26150583
46	С	7,92700984	-1,19608979	0,39127959	7,96275624	-1,23161455	0,25328288	7,96846151	-1,21157814	0,35152086	7,88522039	-1,27801621	0,38347946
47	Η	8,71542859	-1,29196560	1,14402451	8,76424323	-1,38732921	0,98130745	8,75561076	-1,33411010	1,10100341	8,68675242	-1,39120605	1,11945002
48	H	7,38848531	-2,14580937	0,35646253	7,42118497	-2,17506384	0,15393922	7,42319605	-2,15552513	0,28899180	7,31071959	-2,20752861	0,38052467
49	Н	8,40122086	-1,05281582	-0,57871353	8,42043545	-1,01436650	-0,71139232	8,44281568	-1,04120596	-0,61566455	8,33966236	-1,16864850	-0,60064217
50	C	6,42248071	-0,27629636	2,16765147	6,49928422	-0,44113450	2,12586955	6,47861271	-0,33165168	2,15956234	6,43025993	-0,28683631	2,16328011
51	п ц	7,24507855 5 70461112	-0,25522542	2,88884021	7,33727508	-0,46447731	2,82803230	5 76522225	0.42751995	2,87608216	7,25100748	-0,31737078	2,88378928
52	н	5,70461115	-1 24596280	2,45100454	6.01307045	-1 41803420	2,47652605	5,76525525	-1 30081151	2,40057152	5,75776122	-1 22571394	2,45008596
54	C	4.83514429	0.91523504	-2.44603751	4.82752107	1.07233116	-2.37198356	4.87938934	0.96610966	-2.41892846	4.86447508	1.00014568	-2.42116108
55	H	4.19010622	0.04171263	-2.47699972	4.18016125	0.20351086	-2.45022498	4,20759427	0.11306707	-2.44292640	4.13966180	0.19143328	-2.41614600
56	Н	4,20001089	1,80498045	-2,37583172	4,19752985	1,95856493	-2,23908522	4,27343819	1,87734239	-2,35455997	4,31705384	1,94750121	-2,37571147
57	Н	5,36855934	0,98078356	-3,39826436	5,35079745	1,19910491	-3,32322717	5,41879482	1,00745483	-3,36976257	5,38819234	0,98635010	-3,38156052
58	С	2,65172224	-3,10869253	0,08813380	2,68652786	-3,11735677	-0,00680189	2,69603451	-3,11699103	-0,05759801	2,64758666	-3,04015207	-0,00670110
59	Η	1,76865889	-3,70066391	0,31365358	1,81146718	-3,71137547	0,24031098	1,81260822	-3,72948925	0,10209576	1,76970115	-3,65775823	0,15687409
60	Η	3,11263024	-3,52398332	-0,80919923	3,10531191	-3,51587476	-0,93042330	3,17427425	-3,45931601	-0,97552313	3,12656941	-3,38346334	-0,92314318
61	Н	3,37118677	-3,24810963	0,89773360	3,43816229	-3,27527375	0,77005788	3,40220953	-3,31905670	0,75233748	3,35518390	-3,23453627	0,80363839
62	C	-1,04621054	0,88596947	1,00989695	-1,03593482	0,78962835	1,06312870	-1,03884457	0,86288622	1,05614931	-1,09367714	0,94859537	1,04447811
03	н u	-1,580/5827	1,54806384	1,58741370	-1,57587754	1,39110295	1,79072154	-1,58630661	1,51349560	1,/34032/3	-1,64603666	1,63853391	1,67822881
04 65	л Ч	-0,23903514	0,40034920	1,26314840	-0,24016636	0,27039460	1,59/4926/	-0,20442784	0,50721930	1,03500182	-0,32924233	1 54290102	1,00945973
66	0	-0,57294771	-1 03157792	3 63932451	-0,27339561	-1 03890469	3 63774697	-0,54954105 -3 33208006	-1 09780427	3 20385380	-0,59150412	-1.11215222	3 64779210
67	н	-2.82865490	-1.49494454	4.35073601	-2.87264859	-1.49341455	4.34216235	-3.25792283	-1.74423481	2.87991188	-2.81231280	-1.57748506	4.35608893
68	Н	-3,20450097	-1,68394435	2,91658534	-3,26601599	-1,68786080	2,91309863	-2,84125245	-1,55453879	4,30291665	-3,18223612	-1,75937654	2,92098386
69	0	-5,59222086	-0,54001682	-3,15718122	-5,75317912	-0,44624203	-3,15725680	-5,80414535	-0,47997149	-3,19947863	-5,57099017	-0,61239866	-3,20639964
70	Η	-5,11318056	-1,37937175	-3,04181291	-5,31605686	-1,31149798	-3,07420023	-5,29975079	-1,30446994	-3,08615797	-5,09896993	-1,45350025	-3,07871982
71	Н	-6,08674013	-0,50045751	-2,31286855	-6,24589807	-0,41335961	-2,31208465	-6,26124384	-0,42971585	-2,33464367	-6,07165662	-0,55842709	-2,36675842
72	Η	-7,47233445	-3,84282168	-1,56183911	-7,67198149	-3,76153091	-1,52366908	-7,60531320	-3,77391285	-1,52927972	-7,44921189	-3,90821259	-1,53483795
73	Η	-4,43597045	4,66922710	-0,76494272	-4,35303278	4,67245100	-0,65744440	-4,48431493	4,64175203	-0,78364978	-4,49395116	4,64516743	-0,77028716

Table S1b. Cartesian coordinates (in Å) of the QM region of hWT snapshots. Rho_1

model.

	т		hWT1			hWT2			hWT3			hWT4	
Atom	Туре	х	У	Z	х	У	Z	х	У	Z	х	У	Z
1	С	7,69885152	-2,64013818	1,45811297	7,78024052	-2,58806581	1,49660231	7,68592848	-2,65435593	1,46112321	7,67193889	-2,70755696	1,45013677
2	Η	8,17645029	-2,00396911	2,20238815	8,20757686	-1,93847518	2,25922005	8,15205622	-2,01648452	2,21178040	8,11446437	-2,07631303	2,22114424
3	Η	8,46868324	-2,93346380	0,73172435	8,58339103	-2,84704365	0,79435810	8,46185320	-2,93355988	0,73624928	8,47054425	-2,97652100	0,74641945
4	С	6,65547041	-1,82739703	0,67552558	6,72531165	-1,81967899	0,68305382	6,64204365	-1,84667671	0,67325770	6,64402827	-1,89997791	0,63821485
5	0	5,91445668	-2,39450486	-0,15235036	6,03244463	-2,41463724	-0,16488557	5,91345987	-2,41315063	-0,16516176	5,93838063	-2,46843861	-0,21604509
7	C	5 70081445	-0,56951592	0,89732485	5 78222620	-0,56144147	0,90249749	5,03998092	-0,58905101	0,89823680	0,03042902 5 75747604	-0,04155408	0,80004434
8	н	5,23552253	5.02647229	-1.78397209	5,19860855	5.01619762	-1.73916150	5,18055238	5.03733417	-1.69133272	5,17562911	5.07517365	-1.72117578
9	н	6,85802068	5,04168387	-1,12886762	6,83408255	5,04444007	-1,11529241	6,81100666	5,07386613	-1,05995986	6,81099544	5,11802765	-1,09190476
10	С	5,48488176	3,73249808	-0,09195837	5,49928046	3,69395907	-0,07883974	5,48459209	3,69991709	-0,04124148	5,48096071	3,75783046	-0,05682359
11	Н	6,00765432	3,68391790	0,86591425	6,03336530	3,63736318	0,87130785	6,01562151	3,64034981	0,91226818	5,99096656	3,71949048	0,90801334
12	Η	4,41378146	3,67112924	0,12310729	4,43166417	3,61212663	0,14822000	4,41729610	3,60827947	0,18389618	4,40994929	3,66221013	0,14597537
13	С	5,87770606	2,50898991	-0,94574007	5,89800361	2,48853815	-0,95471624	5,89302813	2,50383175	-0,92573299	5,92095810	2,54882031	-0,90904606
14	H	5,58973701	2,68874512	-1,98387112	5,60860657	2,68281729	-1,99101019	5,60951342	2,70727768	-1,96114756	5,67063901	2,73438981	-1,95584810
15	H	6,95620062	2,352/0436	-0,92613383	6,9/6/35//	2,33456924	-0,93923490	6,97200493	2,35108818	-0,90329155	6,99887279	2,40290874	-0,85209956
10	IN H	5,24031247	1,20009259	-0,50839861	5,20133104	1,23302408	-0,53466648	5,25557949	1,24532782	-0,51787834	5,28031298	0.53449146	-0,50435996
18	Ĉ	-7.01997304	-0.00050288	-0.63656571	-7.04292489	-0.08573287	-0.60242360	-7.01110932	0.00221757	-0.64947631	-7.03114144	-0.01229219	-0.63711718
19	č	-7,78308601	1,33835308	-0,63968268	-7,84141891	1,22874272	-0,69825462	-7,78576994	1,33497504	-0,63438025	-7,82500611	1,30784119	-0,59660628
20	Н	-7,18674934	2,07826318	-1,18678211	-7,25141110	1,95328318	-1,27233835	-7,18922906	2,08900897	-1,16237075	-7,24846538	2,07608257	-1,12537105
21	Н	-8,70894537	1,21384932	-1,20735908	-8,75567013	1,05173021	-1,27161353	-8,70770090	1,21321322	-1,20900233	-8,75312998	1,17589769	-1,15856994
22	С	-8,06290927	1,87271088	0,75549689	-8,15614565	1,83058388	0,66226316	-8,07840956	1,83618802	0,77071546	-8,10211078	1,78926131	0,81685933
23	Н	-8,60419521	2,82050961	0,69455207	-8,72729883	2,75575955	0,54434710	-8,63350629	2,77851824	0,73262954	-8,67421737	2,72200447	0,79722698
24	Н	-8,70684639	1,18004124	1,30472721	-8,78489543	1,14774847	1,24090181	-8,71641434	1,12462547	1,30092561	-8,71963729	1,06071897	1,34976478
25	C	-6,75242272	2,07048910	1,51083723	-6,8634/42/	2,11392191	1,42035461	-6,//431981	2,03305792	1,53899315	-6,78898903	1,99983299	1,56357495
20	л н	-6,28108809	3,01526349	2 58279551	-0,42780300	3,00388115	2 48425378	-6,30750023	2,98753132	2 61070081	-0,33978238	2,96190097	2 63965126
28	C	-5.72936593	0.97559880	1.31515782	-5.79497973	1.05360626	1.28755608	-5.74228019	0.95079693	1.33062641	-5.74480727	0.93319791	1.33198818
29	č	-5,80189465	0,07218247	0,30919918	-5,83393993	0,08624931	0,34292023	-5,80079391	0,06773581	0,30551545	-5,80681261	0,05830941	0,30121578
30	С	-4,77412407	-0,94867930	0,08218998	-4,77995893	-0,92135513	0,17815477	-4,76513938	-0,94321697	0,07341954	-4,76285430	-0,93822148	0,04614808
31	Н	-5,12474596	-1,92756148	-0,23124922	-5,11768058	-1,93465240	-0,02435427	-5,10610120	-1,92528172	-0,23922567	-5,09765042	-1,92079111	-0,27332124
32	С	-3,44124873	-0,74219258	0,16003495	-3,45165924	-0,68402455	0,17751831	-3,43493454	-0,72532755	0,15154490	-3,43417480	-0,70731779	0,11652235
33	Н	-3,10333414	0,25936334	0,39229270	-3,12244538	0,33742241	0,32547278	-3,10016423	0,27881831	0,38105113	-3,11109397	0,29870086	0,34951684
34	С	-2,38297413	-1,70636285	-0,03465425	-2,39179825	-1,65208177	-0,00119151	-2,37412881	-1,68992911	-0,03718071	-2,36282998	-1,65834989	-0,07570554
35	С ч	-1,09742895	-1,23/4/866	0,02831006	-1,10543189	-1,18539309	0,01179062	-1,09001753	-1,21799454	0,00541361	-1,082/5539	-1,17641316	-0,00433796
37	C	-0,99013737	-0,17202551	-0.00661260	-0,99094282	-0,11552551	-0.00515667	0 10563174	-0,14942230	-0.01988531	-0,98739314	-0,11067264	-0.03052305
38	н	-0.02270552	-3.07770058	0.15697837	-0.04870747	-3.03070003	0.19844671	-0.01842797	-3.05902940	0.16470311	-0.00136985	-3.01246808	0.12152051
39	С	1,39684655	-1,59336168	-0,12815079	1,38567817	-1,57617590	-0,14294608	1,40185933	-1,58390298	-0,15246832	1,41500846	-1,52584786	-0,14001811
40	Н	2,15712311	-2,35239011	0,02122982	2,13521558	-2,34157342	0,02665194	2,16114133	-2,34240077	0,00036532	2,17296647	-2,28934566	-0,00146868
41	С	1,93245402	-0,31045762	-0,49692866	1,94101746	-0,30876169	-0,54045056	1,94109476	-0,30084669	-0,52476526	1,95456054	-0,23883187	-0,48593101
42	С	3,29238099	-0,13566152	-0,35960331	3,30070562	-0,14689098	-0,39440854	3,30013673	-0,13839998	-0,38697813	3,31869219	-0,08466507	-0,36860361
43	H	3,89537613	-0,94526105	0,04100454	3,88990312	-0,95526701	0,02887822	3,89675034	-0,95265445	0,01057821	3,91636061	-0,91102550	0,00323653
44	C	3,97686115	1,03618236	-0,73967586	4,00073928	1,01596738	-0,78066054	3,99410242	1,03247885	-0,76015331	4,01127453	1,08841035	-0,72673494
45	н	3,45513408	1,82/4418/	-1,27225396	3,49020878	1,80781640	-1,32184/11	3,48011271	1,82963235	-1,29006844	3,49559919	1,89992386	-1,23213670
40	н	-7,93817000	-1,13174731	-0,17514848	-8 73433186	-1,23448021	-0,07302482	-8 71448210	-1,10439031	-0.94286624	-8 72539395	-1 36464235	-0.92049006
48	н	-7.38369080	-2.08730265	-0.08128663	-7.35444577	-2.15175650	0.06600651	-7.35637912	-2.09381330	-0.11917061	-7.34530291	-2.11913274	-0.13203182
49	Н	-8,38975359	-0,94498478	0,79786692	-8,38274956	-0,98589061	0,88643351	-8,38688318	-0,97220975	0,75900497	-8,37123117	-1,02368222	0,77968182
50	С	-6,58688967	-0,26482219	-2,08923065	-6,57980018	-0,43402168	-2,02950166	-6,56745638	-0,23680509	-2,10412217	-6,60560546	-0,22384814	-2,10124339
51	Н	-7,47273419	-0,35235734	-2,72433952	-7,44620473	-0,63949253	-2,66619160	-7,44772278	-0,32625760	-2,74661304	-7,49482268	-0,32131207	-2,73111459
52	Н	-5,99447850	0,57391932	-2,46161331	-6,03558551	0,40205700	-2,47401602	-5,97635343	0,60613801	-2,46702908	-6,04180991	0,64169156	-2,45540403
53	Н	-5,99848897	-1,17315932	-2,20168706	-5,90883825	-1,29393948	-2,04743713	-5,97031462	-1,13892482	-2,22211744	-5,99105943	-1,11057062	-2,24162353
54	C	-4,64678491	0,99941601	2,35985893	-4,/1545295	1,19006661	2,32619937	-4,66691927	0,96214588	2,38243743	-4,65/01//3	0,95/124/9	2,3/242161
55 56	л н	-4,11329022	1 7795013319	2,44511223	-4,07654130	2 05/90118	2,411/7275	-4,12238030	1 75740741	2,44908021	-4,07836103	1 78308439	2,41203260
57	н	-5 08903839	1 22361022	3 33292829	-5 18042483	1 36678775	3 29941053	-5 11832187	1 16039088	3 35797667	-5,50050057	1 11998756	3 35667445
58	c	-2.73371271	-3.14482991	-0.27937105	-2.75031448	-3.09772949	-0.19018390	-2.72724275	-3.13055487	-0.26339585	-2.69747536	-3.09948254	-0.32593639
59	Ĥ	-1,86358363	-3,74215460	-0,54574441	-1,88466160	-3,70857249	-0,43753206	-1,85248508	-3,74150385	-0,47842733	-1,81804591	-3,69275317	-0,56443791
60	Н	-3,16346015	-3,58163293	0,62616826	-3,18469604	-3,50432180	0,72490055	-3,19816300	-3,54345093	0,63047503	-3,15093031	-3,53548768	0,56757764
61	Н	-3,47077910	-3,23813672	-1,08128449	-3,48648820	-3,21542215	-0,99029943	-3,42944014	-3,23421214	-1,09477734	-3,41283925	-3,19898588	-1,14599662
62	С	1,03901974	0,76981636	-1,04996179	1,06140165	0,76410403	-1,13189329	1,04997730	0,78126838	-1,07896196	1,06189212	0,86548664	-0,98975347
63	Η	0,58648119	1,35203132	-0,24378577	0,56183871	1,33555917	-0,34540802	0,56010307	1,33495736	-0,27253965	0,57677604	1,38252027	-0,15671098
64	Н	1,57942801	1,46696264	-1,68717929	1,62082973	1,47308773	-1,73911114	1,59988196	1,50311965	-1,67852997	1,60687372	1,61514312	-1,55828790
65	н	0,23125679	0,33766180	-1,63781862	0,28958191	0,32309088	-1,76140331	0,26965258	0,35333056	-1,70617622	0,27763065	0,46427852	-1,62951294
00 67	н	3,52209/35	-1,51465404	-3,40118642	3,50988399	-1,48544037	-3,51186403	3,55608830	-1,382/8388	-3,4/240341	3,42580505	-1,4/86/207	-3,48648159
68	н	3,46200327	-1,04705569	-2.75566337	3,44406852	-2.1710/220	-7,81607428	2,00449377	-2.08348820	-2.78992752	2,74303301	-2.17977867	-2,80572374
69	0	5,60923936	-0.11308696	3,40966754	5,71910593	-0.14643575	3,45805559	5,57550749	-0.12322627	3,40069275	5,67857291	-0.25548572	3,42718043
70	H	5,07559636	-0,91665711	3,30003950	5,19490154	-0,95914043	3,36522249	5,07308965	-0,94840897	3,30808616	5,13316849	-1,05048603	3,32548144
71	Н	6,11284677	-0,15227644	2,56225625	6,18722834	-0,17147416	2,59134997	6,09007722	-0,16619774	2,56142547	6,13566568	-0,27551476	2,55424849
72	Н	7,40682982	-3,57847893	1,92800034	7,51719619	-3,54227593	1,95248379	7,40962710	-3,60386721	1,92179126	7,38576015	-3,66079376	1,89530922
73	Н	5,59762879	5,96881970	-0,34210146	5,57371003	5,93342790	-0,28599498	5,54057639	5,93883794	-0,21997582	5,53770804	5,99516166	-0,26598977

Table S1c. Cartesian coordinates (in Å) of the QM region of hM207R snapshots.

Rho1 model.

	-		hM207R1			hM207R2			hM207R3			hM207R4	
Atom	Type	х	У	Z	х	У	Z	х	У	Z	х	У	Z
1	С	7,46154003	-2,98584945	0,77104201	7,53865845	-2,91029465	0,91891900	7,38202686	-2,99951435	0,88737402	7,40783192	-2,91448724	1,02007611
2	Н	8,39325754	-2,82427149	0,21330980	8,47410820	-2,77085657	0,36150263	8,31903641	-2,88227298	0,32796028	8,33640480	-2,81528925	0,44234401
3	Н	7,07045782	-3,95154482	0,45327271	7,14968487	-3,88987651	0,64127157	6,96717094	-3,96317484	0,59586383	7,00332444	-3,89837897	0,78762629
4	С	6,49664469	-1,86008614	0,35433433	6,57322542	-1,80616109	0,44639120	6,44846659	-1,86466049	0,42502750	6,45176770	-1,81859642	0,51509109
5	0	5,58250639	-2,14973630	-0,44153263	5,63517873	-2,14338689	-0,30386768	5,55385583	-2,16391797	-0,39244284	5,53893631	-2,16869910	-0,25861505
6	0	6,69277587	-0,67773958	0,79989401	6,78977221	-0,59595886	0,79695117	6,64895994	-0,67535353	0,84763444	6,65083101	-0,60462642	0,86195111
8	н	4,78076280	4,24934462	0,32041877	4,65958643	4,25608671	0,15149890	4,63521932	4,2/452/26	0,26422863	4,62313415	4,23106687	0,17232507
9	н	4 24567829	4 31581842	-0.62986328	4 14127882	4 28369720	-0.80966190	4 12330165	4 34023071	-0 69850889	4,07720310	4 23474722	-0 77115192
10	C	6.17249833	3.65397121	0.10716759	6.07003871	3.68435153	-0.02621324	6.05607885	3.73147423	0.08779479	6.04368240	3,70099157	-0.04781164
11	Н	6,86022396	4,38530854	-0,33141229	6,74601285	4,41795030	-0,47854603	6,72173557	4,48841536	-0,34153076	6,68765915	4,45915035	-0,50635979
12	Н	6,61675898	3,34844649	1,05875222	6,50937447	3,42174852	0,94119047	6,48961324	3,45952083	1,05511763	6,51243285	3,43980288	0,90484712
13	С	6,18105412	2,47167377	-0,86949403	6,12340735	2,46843880	-0,96355011	6,14821671	2,53503652	-0,86985065	6,10475697	2,49855529	-1,00136460
14	Н	5,83524858	2,79308722	-1,85463670	5,77403341	2,74483390	-1,95954850	5,82596634	2,82537257	-1,87158208	5,74083072	2,78237846	-1,98973865
15	Н	7,19624267	2,09981778	-0,98862632	7,15102607	2,12423804	-1,06713015	7,18078281	2,20067960	-0,95384984	7,13541364	2,16833393	-1,12357284
16	N	5,35822816	1,32696465	-0,45181142	5,33439491	1,31042936	-0,51508621	5,35547850	1,36465990	-0,46322795	5,32955093	1,33631813	-0,55222686
17	Н	5,84814051	0,52258814	0,05089474	5,84927803	0,54200483	0,01996550	5,84453416	0,57292582	0,05291921	5,82612552	0,57650815	0,00498824
18	C	-6,801/9/39	0,33458418	-0,92597591	-6,/99529/6	0,21256997	-0,95384845	-6,///32141	0,30864717	-0,90708930	-6,75399485	0,27534558	-0,90864707
20	н	-7,82368/13	2 37272560	-0,50564996	-7,81312311	2 20//7/57	-0,66261459	-7,70040124	2 36776092	-0,49279899	-7,72429055	2 36075110	-0,55199642
20	н	-8 58844245	1 49086453	-1 28536685	-8 57219041	1 33818322	-1 45083498	-8 52806899	1 52169176	-1 26453497	-8 50308463	1 47431558	-1 31734460
22	Ċ	-8.45740716	1,13673801	0.85261442	-8.44929291	1.23932904	0.71585161	-8.38581990	1.19289272	0.87603111	-8.33034815	1.28501423	0.83787275
23	Н	-9,19936203	1,90452339	1,08951475	-9,18491268	2,03460709	0,85923064	-9,09714117	1,98880199	1,10818980	-9,03285498	2,10264518	1,02633504
24	Н	-8,99313837	0,18318683	0,85689977	-8,99417836	0,29746657	0,82810645	-8,95661128	0,25997661	0,89645032	-8,91003521	0,36251173	0,92832310
25	С	-7,37130155	1,12452839	1,92093128	-7,36316735	1,33614487	1,77678673	-7,29054947	1,15927693	1,93454938	-7,22157963	1,31143159	1,88133710
26	Η	-7,04709888	2,15152705	2,14684181	-7,03033195	2,37831116	1,88985379	-6,95178713	2,18019559	2,16609069	-6,85561636	2,33934361	2,02446974
27	Н	-7,76337902	0,73028535	2,86204542	-7,76091179	1,05294196	2,75578911	-7,68234743	0,76475640	2,87663488	-7,60779372	1,00253659	2,85710334
28	С	-6,14064847	0,33696792	1,54292089	-6,13654454	0,50208271	1,49700446	-6,06875334	0,35910946	1,54851610	-6,02900101	0,45135541	1,53872876
29	С	-5,87307042	-0,03876888	0,26103551	-5,86515102	-0,01844236	0,26680713	-5,82636423	-0,04335100	0,26961251	-5,81192033	-0,03377701	0,28460404
30	С н	-4,69233695	-0,83475445	-0,10769851	-4,68332321	-0,85088710	-0,00984635	-4,65095189	-0,84411258	-0,10905884	-4,66132559	-0,88554942	-0,05097575
32	C	-4,84990002	-1,33239109	-0,92008034	-4,05145551	-1,00843029	0,77602099	-4,01015552	-1,52601662	-0,94061281	-4,03530500	-1,03324000	0 30073635
33	н	-3 21198908	0.00454570	1 11320694	-3 20739277	0.06591608	1 16425242	-3 16283066	-0.00964378	1 10371430	-3 14633118	0.05431166	1 04141967
34	c	-2.30556182	-1.59921954	0.01208689	-2.30232121	-1.61968230	0.19295007	-2.26145818	-1.61027799	0.00496024	-2.27097626	-1.64063251	0.06856319
35	С	-1,04935308	-1,10410414	0,21742959	-1,04368110	-1,10769366	0,31782994	-1,00680927	-1,11130416	0,20228866	-1,01353649	-1,12685407	0,20058297
36	Н	-0,97071027	-0,10879776	0,63929413	-0,95540599	-0,07550011	0,63514392	-0,92868757	-0,10830338	0,60537130	-0,93330308	-0,09211456	0,51291918
37	С	0,16766830	-1,82317924	-0,04895224	0,16980157	-1,84872361	0,08340566	0,21195085	-1,83921862	-0,03539946	0,20481185	-1,86996711	0,02268515
38	Н	0,05917699	-2,90421009	-0,06044693	0,06676774	-2,92525230	0,18497424	0,11193396	-2,91977134	0,01878186	0,10662821	-2,94440250	0,15026945
39	С	1,43945305	-1,37537659	-0,23320922	1,43422019	-1,42041553	-0,17742575	1,47698981	-1,38878493	-0,24393053	1,46934643	-1,42713246	-0,19971102
40	н	2,19663232	-2,14619450	-0,31364223	2,19108701	-2,19665373	-0,19840360	2,24415299	-2,15391843	-0,27445207	2,24402026	-2,18564170	-0,16907846
41	C	1,98205728	-0,03899767	-0,40367434	1,97597898	-0,10218425	-0,46220816	2,004/2296	-0,05538574	-0,47533629	1,9868/663	-0,10/28333	-0,51112567
42	н	3,34473803	0,04859095	-0,41742419	3,33893860	-0,00625444	-0,45050550	3,30501502	-0.82951437	-0,45278365	3,34099524	-0.84223274	-0,47237766
44	c	4 09402359	1 22422044	-0 71821090	4 07843960	1 16399867	-0.80232740	4 09964108	1 23097118	-0 75850737	4 07297706	1 18074725	-0.83934536
45	Н	3,63366094	2,06261655	-1,23301998	3,61365318	1,97066525	-1,36223613	3,63632772	2,05534058	-1,29280036	3,60524161	1,97638780	-1,41089487
46	С	-7,56609026	-0,89566847	-1,46413865	-7,57506707	-1,07100816	-1,32720267	-7,58063899	-0,92311319	-1,38015133	-7,56766705	-0,96851577	-1,33083646
47	Н	-8,30757258	-0,58347870	-2,20346656	-8,33003128	-0,84869644	-2,08443430	-8,32442222	-0,62350606	-2,12213461	-8,29535795	-0,70204598	-2,09969925
48	Η	-6,90164139	-1,58367554	-2,00222705	-6,92261628	-1,82120504	-1,78970648	-6,94301257	-1,65607187	-1,88816742	-6,93053103	-1,73149708	-1,79507600
49	Н	-8,10704361	-1,42774846	-0,67773062	-8,09917792	-1,50358099	-0,47061013	-8,11523866	-1,41097850	-0,56142073	-8,12858552	-1,40019855	-0,49765543
50	С	-5,96084076	0,90833060	-2,08407193	-5,97439839	0,63883687	-2,18329471	-5,95877284	0,82584650	-2,10900340	-5,91552435	0,72442748	-2,12295429
51	п	-0,00594842	1,17903244	-2,91950453	-0,03404842	0,78788467	-3,04085388	-0,02950039	1,10923964	-2,92054674	-0,57050333	0,98550595	-2,95392109
52	н	-5,429/1111	1,81083924	-1,///9/123	-5,45870198	1,58283073	-2,00117654	-5,37547584	1,70815820	-1,84349288	-5,32130455	-0.05203426	-1,88044043
54	ĉ	-5,24884758	0,04030578	2,72322641	-5,24613713	0,34843047	2,70525277	-5,15753962	0,08632363	2,72136211	-5,11328320	0,21659499	2,71546952
55	Н	-4,64963865	-0,86174316	2,60566132	-4,65815327	-0,56872166	2,70562474	-4,56914764	-0,82502458	2,61899264	-4,55056235	-0,71399059	2,65351870
56	Н	-4,55523465	0,87167574	2,88161292	-4,54217713	1,18677718	2,75445932	-4,44854173	0,91168034	2,84596335	-4,38336379	1,02917290	2,78965155
57	Н	-5,84580620	-0,06299584	3,63034293	-5,84351269	0,37246043	3,61732687	-5,73823738	0,01515996	3,64201786	-5,68553926	0,20791213	3,64362189
58	С	-2,52844347	-2,96097598	-0,59904607	-2,52883422	-3,03804367	-0,26939747	-2,47483295	-2,98351968	-0,58387573	-2,50160117	-3,05994033	-0,38856131
59	Н	-2,10394458	-3,03522881	-1,60749904	-2,11871076	-3,22089672	-1,26939132	-2,00486721	-3,08799319	-1,56749185	-2,04005479	-3,25919174	-1,36144311
60	Н	-2,05544346	-3,72984292	0,01770413	-2,04475561	-3,73452158	0,42026593	-2,04401784	-3,73715011	0,08008941	-2,07110668	-3,75139011	0,34024723
61	н	-3,58587231	-3,21506734	-0,64/03573	-3,58624318	-3,29627904	-0,2/418854	-3,53163112	-3,22530053	-0,68301622	-3,56209864	-3,29985762	-0,45352280
62	ц	1,09255654	1,10515012	-0,55205846	1,07906811	1,07879383	-0,72182134	1,10326902	1,124/0831	-0,71449563	1,07890260	1,04391326	-0,84069223
64	н	0,05440355	2 04330117	-0.800328890	1 60080350	1 91100380	-1 18068642	0,05211944	1 98241121	-1 12180210	0,36829810	1,42820443	-1 30028129
65	н	0.28402928	0.97317050	-1.25716318	0.25282792	0.80975004	-1.37840244	0.30665714	0.86802246	-1.41204568	0.29877761	0.73380280	-1.54037565
66	0	3,74122143	-0,57374151	-3,58579511	3,82130706	-0,85635386	-3,54605520	3,67923233	-0,69605776	-3,66399318	3,60163185	-0,92366808	-3,59045489
67	Н	2,99084530	-0,63993684	-4,19542859	3,05600713	-0,99346108	-4,12195777	2,90678431	-0,78308388	-4,24151952	2,80872678	-1,02921498	-4,13819164
68	н	3,63525169	-1,37526600	-3,04203500	3,74236015	-1,59784526	-2,91645927	3,58202415	-1,46397920	-3,07149983	3,52234811	-1,67124253	-2,96869878
69	0	6,04722011	-0,40902271	3,51540763	5,97667337	-0,07545255	3,42971676	5,92355160	-0,34073403	3,55788439	5,90650214	-0,03242974	3,50428562
70	Н	5,41896702	-1,14151939	3,42609480	5,41092056	-0,86316186	3,40099514	5,30310815	-1,08171540	3,47506730	5,31337097	-0,80022108	3,50067366
71	Н	6,39428524	-0,41069472	2,59115108	6,39254637	-0,17285591	2,53914090	6,29366298	-0,36673385	2,64367995	6,29159750	-0,15142952	2,60309711
72	H	7,74134683	-3,02559691	1,82393017	7,81858375	-2,91048402	1,97222617	7,65860219	-3,01622751	1,94112775	7,70087943	-2,87109790	2,06922182
73	н	4,//194612	5,24437306	0,76542984	4,61972677	5,26167528	0,56924524	4,58546577	5,26140761	0,72573263	4,5/401713	5,24158486	0,57763863

Table S1d. Cartesian coordinates (in Å) of the QM region of hS186W snapshots.

Rho1 model.

	-		hS186W1			hS186W2			hS186W3			hS186W4	
Atom	Туре	х	У	Z	х	У	Z	х	у	Z	х	у	Z
1	С	8,52400618	-4,29563252	0,21739502	8,28396196	-4,43011539	0,23351035	8,30258106	-4,41139003	0,11789868	8,25453573	-4,39170011	0,11561799
2	Н	9,58752058	-4,05698172	0,21941468	9,34833929	-4,19133006	0,23266568	9,37081609	-4,19577402	0,14074267	9,31691711	-4,15312662	0,15991986
3	Н	8,37851291	-5,12452012	-0,47688032	8,14020334	-5,25935983	-0,45999402	8,15331661	-5,22631599	-0,59364118	8,13716448	-5,21212706	-0,59484721
4	С	7,83893114	-3,08121827	-0,36677240	7,60113534	-3,21675979	-0,35556464	7,65711896	-3,17395160	-0,46257626	7,59402341	-3,17044852	-0,48165616
5	0	8,46491904	-2,13570869	-0,81074194	8,23507016	-2,28885564	-0,82485639	8,31397562	-2,24889849	-0,90349615	8,24030187	-2,24337574	-0,93534045
6	0	6,50616104	-3,16097985	-0,44296496	6,26798550	-3,28099194	-0,41348654	6,32423932	-3,21227115	-0,53827101	6,26145249	-3,21848832	-0,55412759
,	U U	6,11236522	-2,42826258	-0,95989761	5,87885221	-2,55222593	-0,93906199	5,94365578	-2,46/41423	-1,04691379	5,87622045	-2,48240841	-1,0/150635
0	п	4,00536535	3,98039349	2,53860564	4,15659809	2 92224574	2,48524191	3,99504526	2 01200021	2,55985589	4,00111270	3,93257591	2,60498030
10	C	3,97002330	4 31244435	2,38587333	3 17166632	4 32629063	2,33732740	3,02690200	4 39041115	2,37307004	3,02151518	4 29048100	2,00073839
11	н	5.06385976	4.46942071	1.53759632	5.20791967	4.48804763	1.47081587	5.05607637	4.45053785	1.54463388	5.05768658	4,44136310	1.61490071
12	Н	5,32908091	5,51817521	1,69427719	5,46768826	5,53978929	1,60128406	5,42891639	5,45639699	1,74499318	5,35715260	5,46966140	1,82853091
13	С	5,98779504	3,91126453	1,64258399	6,13814583	3,94125255	1,58188179	5,92657706	3,80491366	1,57233158	5,96665975	3,85124202	1,67113274
14	Н	4,62432108	4,39177660	0,06629673	4,75536406	4,37633230	0,00772617	4,54632923	4,47881108	0,09512885	4,59352637	4,45992438	0,14909031
15	Н	3,73009628	5,01065418	-0,05887009	3,86775780	5,00188035	-0,12739213	3,64410302	5,09705098	0,04833686	3,69823706	5,08564409	0,07203788
16	Ν	5,41242205	4,82063558	-0,55465179	5,54242523	4,77834672	-0,63269814	5,30346911	4,93531689	-0,54342643	5,37218166	4,91727723	-0,46357067
17	Н	4,36657755	3,03510261	-0,40596409	4,47518775	3,01063994	-0,41316328	4,26548457	3,14369508	-0,41417839	4,32131766	3,12984228	-0,37376088
18	С	-6,85962715	0,21027037	-0,79611512	-6,86699192	0,14965717	-0,85632903	-6,75259925	0,34803527	-0,79567098	-6,75136468	0,29349714	-0,82174410
19	C	-7,73487357	1,19078519	0,00918218	-7,72084413	1,20354440	-0,12464841	-7,64594644	1,22033339	0,10934623	-7,69159412	1,15887090	0,04241517
20	н	-7,11959680	2,04543016	0,31352673	-7,08563076	2,06726029	0,11120756	-7,03170395	2,01895000	0,54457014	-7,11604009	1,99471447	0,45905922
21	С	-8,52023574	1,58/505/3	1 24820066	-8,50154008	1,50033045	1 16020006	-8,40525058	1,/101/414	-0,50630576	-8,45924810	1,00205447	-0,60021206
23	н	-8,94504187	1 27376687	1,24820300	-8,33020391	1 44285462	1,10023030	-8,23710742	1 08092318	1,23377113	-8,33112703	1 03042930	1,18581519
24	н	-9.00628784	-0.27083253	0.95705090	-9.02523657	-0.14854710	0.92775294	-8.94995354	-0.34614210	0.82108479	-8.94866214	-0.43105062	0.79088378
25	C	-7,24535090	0,01965236	2,16418644	-7,25412588	0,16956897	2,11179852	-7,23126309	-0,21517015	2,11110851	-7,25168521	-0,18892242	2,09559717
26	Н	-6,83416976	0,83704014	2,77408929	-6,85166880	1,00473053	2,70189058	-6,81607576	0,53199323	2,80332780	-6,87421207	0,59677260	2,76738845
27	Н	-7,66964718	-0,69162052	2,88064210	-7,69381566	-0,51602387	2,84320304	-7,68197976	-0,98608425	2,74355779	-7,67755341	-0,95371495	2,75124789
28	С	-6,08710245	-0,64921518	1,46259959	-6,08238224	-0,52183035	1,45730321	-6,07373596	-0,82375828	1,35876758	-6,06054352	-0,77976819	1,37794193
29	С	-5,87187749	-0,52961066	0,13439657	-5,86287920	-0,49587506	0,12513730	-5,81848457	-0,54105936	0,06070852	-5,79241677	-0,52884949	0,07467061
30	С	-4,72051108	-1,14139879	-0,54387550	-4,68974548	-1,12558843	-0,49592283	-4,65114511	-1,06874272	-0,65255382	-4,59857853	-1,03639911	-0,60964577
31	Н	-4,92575476	-1,63316307	-1,49180963	-4,87220868	-1,69035268	-1,40641155	-4,80796126	-1,33248100	-1,69441801	-4,73277857	-1,29928597	-1,65433234
32	С	-3,44311950	-1,05738931	-0,12650820	-3,41938606	-0,98418913	-0,06901365	-3,40142354	-1,14101344	-0,15449837	-3,35426794	-1,10484577	-0,09196198
33	н	-3,250/141/	-0,50620081	0,78534354	-3,24/90166	-0,35853626	0,79970136	-3,2419118/	-0,80970063	0,86427002	-3,21109467	-0,78155911	0,93106018
34	C	-2,26210907	-1,56163999	-0,80118436	-2,22163292	-1,52485410	-0,68083971	-2,19386971	-1,51314703	-0,863/5124	-2,13041416	-1,47593912	-0,77760472
36	н	-1.06140379	-0.51632282	0.52630819	-1.05296790	-0 34532079	0 56407270	-1 02296009	-0.72390639	0.66573774	-0,97027678	-0 77440015	0.81357534
37	C	0.25859980	-1.46634940	-0.87939865	0.28882675	-1.42075925	-0.73861911	0.31297841	-1.44314352	-0.87904768	0.37067167	-1.47769424	-0.74830347
38	Н	0,36992439	-2,43638407	-1,35857373	0,38799907	-2,41859379	-1,16064428	0,42190734	-2,35473840	-1,46170662	0,49668645	-2,44011803	-1,23862061
39	Ċ	1,38456142	-0,70585649	-0,84644030	1,42831603	-0,67994599	-0,73902946	1,43029832	-0,67699522	-0,79661406	1,46642284	-0,68186523	-0,74501138
40	Н	2,28952965	-1,17031998	-1,22622884	2,32726262	-1,18046786	-1,08837467	2,32065708	-1,06685598	-1,27958823	2,36984854	-1,10011338	-1,17836996
41	С	1,57730247	0,68091774	-0,44814336	1,63785182	0,71996335	-0,41006453	1,61775826	0,65642998	-0,24106359	1,61646764	0,69952667	-0,30982026
42	С	2,82186455	1,21859607	-0,60453549	2,90075607	1,21776742	-0,54300900	2,76051291	1,31080580	-0,58378997	2,81002100	1,30224067	-0,56148569
43	Н	3,61793558	0,60331354	-1,01412372	3,69419822	0,56376069	-0,88931802	3,49769618	0,79752945	-1,19542988	3,59358327	0,73667934	-1,05633893
44	C	3,18790362	2,56905158	-0,24506834	3,28669005	2,57513734	-0,24314871	3,10534541	2,65856894	-0,19731436	3,15283735	2,65296516	-0,18632492
45	н	2,41/15808	3,19552293	0,20846793	2,52262995	3,23/33/32	0,17182302	2,34524066	3,26265110	0,30332594	2,38653219	3,25796328	0,30353513
40	н	-7,74530403 9,27600262	-0,65540956	2 25055572	-7,70914785 9.42170747	-0,95195004	2 2161 2921	-7,02004640 9,02004640	-0,54809704	-1,09710342	-7,37923329 9.34977104	-0,00341239	-1,70474115
48	н	-7.12701285	-1.57416480	-2.01695695	-7.16797482	-1.73012735	-1.92326912	-7.01060761	-1.15191735	-2.36548261	-6.93693947	-1.26869147	-2.34885984
49	н	-8.38397132	-1.36973559	-0.80682861	-8.38410976	-1.43145660	-0.68856027	-8.24758272	-1.22849273	-1.11308359	-8.18471815	-1.34802863	-1.10694015
50	С	-6,11275247	1,03120808	-1,86674988	-6,14484627	0,86462707	-2,01580911	-5,94106895	1,30116534	-1,69761773	-5,97362552	1,25230418	-1,74724515
51	Н	-6,83343219	1,58239030	-2,47768773	-6,87622458	1,36891377	-2,65288513	-6,62336999	1,94876484	-2,25321321	-6,67842183	1,86383795	-2,31738704
52	Н	-5,43872364	1,75743996	-1,40679271	-5,44946212	1,61972425	-1,64394044	-5,28331376	1,94127303	-1,10422120	-5,34367774	1,93217764	-1,16883691
53	Н	-5,52310788	0,40444822	-2,53898313	-5,58357136	0,17332226	-2,64713259	-5,32837430	0,77319579	-2,43103075	-5,34015607	0,73029927	-2,46569175
54	С	-5,22956546	-1,45843133	2,40149568	-5,21585367	-1,24289967	2,45703850	-5,24850189	-1,75754438	2,20824127	-5,22510758	-1,66290497	2,27098648
55	H	-4,56269383	-2,15095946	1,89145529	-4,52292899	-1,94613782	2,00391416	-4,68239412	-2,48366757	1,62776881	-4,61759564	-2,37944781	1,72138955
50	H	-4,62348153	-0,80101966	3,03690448	-4,63938638	-0,52/32396	3,05675764	-4,5421/583	-1,19611003	2,83140989	-4,55873866	-1,06310205	2,90222661
59	п С	-5,87800918	-2,03761203	3,06449468	-3,80001820	-1,79599982	3,14813500	-5,90844967	-2,30468292	2,88505108	-3,88189815	-2,22203095	2,94047819
50	н	-1 47591459	-2 77614864	-2,01809599	-1 39995065	-2 93402336	-2.09214512	-1 33984397	-2,14771210	-2 73234009	-1 22702053	-1 93843415	-2,10000032
60	н	-3 06312431	-3 28639226	-1 79710951	-3 04358370	-3 30070859	-1 55402724	-2 63816608	-3 18153246	-2 11228857	-2 39064520	-3 13057833	-2 10591064
61	Н	-2.91973523	-1.86488476	-2.82658436	-2,75784224	-1.99780355	-2.70805531	-3.01032957	-1.62961142	-2,86241781	-2.95128642	-1.60264739	-2.78310702
62	С	0,42358962	1,49778801	0,07983294	0,48306920	1,59611099	0,00779520	0,58305628	1,26945167	0,66891090	0,48678770	1,41889972	0,38307224
63	Н	0,61395466	2,56525311	0,03710598	0,70037083	2,65456966	-0,10200197	0,86732517	2,25646258	1,01958289	0,61029331	2,49740819	0,37651418
64	Н	-0,47639142	1,30629291	-0,50139759	-0,39220160	1,38296905	-0,60118815	-0,38244841	1,35550376	0,17178123	-0,46480365	1,19614005	-0,09450728
65	Н	0,21257824	1,24030502	1,12165197	0,20935031	1,41956485	1,05229107	0,44304345	0,64366826	1,55481083	0,40694354	1,09842287	1,42680290
66	0	5,35491170	3,32844835	-3,01166057	5,45012804	3,30124334	-3,01420754	5,42076071	3,49120113	-2,90507978	5,24083156	3,39465408	-3,02167158
67	H	6,08375901	2,74915947	-3,25269186	6,11839006	2,67236570	-3,30061273	5,10563900	3,13629758	-2,07016008	5,00638467	3,09713561	-2,13827781
68	Н	5,09282101	3,00017593	-2,13149476	5,18756149	2,96316520	-2,13804482	6,09009368	2,84229031	-3,18463890	5,95073776	2,77890307	-3,28168703
69 70	U U	5,77380640	-2,88/53146	3,35023486	5,60340164	-2,89/13200	3,18942713	5,57539461	-3,00925379	3,33/81296	5,57553495	-2,98042912	3,30038942
70	п	5,30209955 5,3752023	-3,05008/5/	2,91034226	5,245/6413	-2,80480184	4,09248268	5,00771564	-2,835/1541	4,10/24206	5,11004822	-3,09331863	2,82914234
72	н	8.26064128	-4.64199887	1.21701370	8.02570203	-4.78198515	1.23238105	8.00954397	-4.76865081	1.10584359	7,95225233	-4.74812679	1.10038750
73	Н	4,13290177	4,34813981	3,55866409	4,26774985	4,40989738	3,49837105	4,14953121	4,32134525	3,59029804	4,14308865	4,24565217	3,63915208

Table S2. Cartesian coordinates (in Å) of the QM region of hWT, hM207R and hS186W. **Rho₂** model.

	<i>m</i>		hWT			hM207R			hS186W	
Atom	Туре	х	у	Z	х	у	Z	х	у	Z
1	С	-8,12401856	3,32726013	0,51551448	6,94401066	-2,85591434	-0,06455362	6,78466967	-2,81676443	-0,68196215
2	н	-7,57706492	3,37820860	1,45965944	6,30299867	-2,43097634	-0,84047321	6,33260117	-2,11816865	-1,38904737
3	н	-9,17537199	3,17727209	0,78040572	6,38955323	-2,79438571	0,87422449	5,99397885	-3,08453681	0,02176676
4	С	-7,60714357	2,12994929	-0,28458285	8,24656886	-2,06267111	0,05156418	7,93805355	-2,15555699	0,07769482
5	н	-8,10092214	2,04335986	-1,25396568	9,02344832	-2,63200328	0,57106535	8,54883046	-2,89052135	0,60862971
6	н	-6,53718030	2,24211227	-0,48276103	8,64848094	-1,82284338	-0,93619118	8,60441715	-1,65842840	-0,61650052
7	С	-7,83636289	0,82518975	0,50004552	8,06197432	-0,77205736	0,86051114	7,49127809	-1,14188309	1,13577278
8	н	-7,62012762	0,98662026	1,55998088	7,71171190	-1,02866570	1,86507776	6,85834485	-1,65358686	1,87339467
9	н	-8,87331428	0,50379495	0,42485577	9,00817293	-0,24373675	0,96155292	8,37721495	-0,77149311	1,65886939
10	N	-7,01385946	-0,29381264	0,02997517	7,12345006	0,18365980	0,27158948	6,80664238	-0,00886945	0,55988726
11	н	-7,53062411	-1,08662112	-0,46681882	7,56514679	1,02296006	-0,21880153	-4,84087314	-0,41405039	1,13941375
12	С	5,23967968	0,23550132	0,94928467	-5,19210194	-0,28973034	1,12131332	-5,23941594	-1,89455321	1,28141500
13	С	5,86257556	1,61667620	1,22621317	-5,91390941	-1,65048548	1,12519055	-4,34211288	-2,47352171	1,52859644
14	н	5,12771022	2,23348181	1,75679994	-5,19334216	-2,42204213	1,41371767	-5,92088243	-1,99908892	2,13150422
15	н	6,70952073	1,48916680	1,90666377	-6,67951231	-1,63497905	1,90523929	-5,86955488	-2,45857752	0,01560431
16	С	6,28546783	2,33692346	-0,04320353	-6,51060846	-2,01132112	-0,22620255	-6,12922374	-3,51128777	0,15694213
17	н	6,74454936	3,30027756	0,19444501	-7,03651634	-2,96838238	-0,17338377	-6,80987740	-1,94073302	-0,19211889
18	н	7,04867805	1,75614964	-0,56882977	-7,25487287	-1,26666413	-0,52132839	-4,92590633	-2,31008171	-1,17476780
19	С	5,07995326	2,54266893	-0,95278746	-5,40288929	-2,07909091	-1,27147267	-4,23216982	-3,16084155	-1,21145581
20	н	4,49211301	3,40334162	-0,60310394	-4,87643445	-3,04181858	-1,19116820	-5,49413447	-2,37375978	-2,10908770
21	н	5,41023670	2,81437761	-1,96051167	-5,83049668	-2,07397668	-2,27937265	-4,09675391	-1,04731725	-1,19807624
22	С	4,14792792	1,35856493	-1,05203804	-4,36218770	-0,98581372	-1,17235640	-4,00217690	-0,21033687	-0,14161486
23	С	4,18473438	0,32885119	-0,17640629	-4,20895363	-0,20727333	-0,07271469	-3,14663571	0,98330412	-0,12959357
24	С	3,27405384	-0,81796376	-0,24047667	-3,17544294	0,82846951	0,01874515	-3,55984818	1,87115564	0,34038443
25	н	3,72048544	-1,78265403	-0,01976319	-3,46171714	1,72119851	0,56451069	-1,86875359	1,01002028	-0,54709316
26	С	1,94147075	-0,77498630	-0,44200035	-1,91551384	0,77510754	-0,46971362	-1,45722592	0,09711641	-0,95798790
27	н	1,47313527	0,19053377	-0,58848707	-1,58148299	-0,14541304	-0,92902650	-0,92080905	2,09850488	-0,43723539
28	С	1,03479159	-1,90121992	-0,40727499	-0,89620700	1,80122475	-0,39709117	0,37352524	1,82574087	-0,74990818
29	С	-0,30638184	-1,63881840	-0,47159745	0,39841885	1,44387256	-0,65626986	0,57102028	0,81643369	-1,08191783
30	н	-0,58147206	-0,59705558	-0,57097021	0,58498789	0,40019710	-0,87619836	1,50492293	2,71429179	-0,67052816
31	С	-1,36006189	-2,60256318	-0,45768403	1,50771917	2,34767616	-0,67399788	1,29458323	3,77653029	-0,75697358
32	н	-1,06300644	-3,63357344	-0,61916762	1,25375275	3,39127955	-0,83398931	2,81120622	2,39537171	-0,49007604
33	С	-2,70830699	-2,42613107	-0,34032698	2,84644054	2,11970954	-0,55764835	3,50694574	3,22840718	-0,51478679
34	н	-3,30499429	-3,30929605	-0,51823698	3,48909626	2,97547370	-0,73207363	3,44094343	1,12959601	-0,15229291
35	C	-3,48633857	-1,2/152486	0,01569125	3,56282332	0,94354135	-0,14589307	4,77016610	1,13685740	0,11636372
30	C	-4,85168134	-1,35645017	-0,15420381	4,93584455	1,03324948	-0,18569782	5,33776741	2,04953388	-0,03239241
37	н	-5,29553145	-2,24833436	-0,58665218	5,37854729	1,91965157	-0,61880832	5,53661614	0,01949052	0,62827864
38	C II	-5,72866229	-0,32094623	0,22420441	5,82555707	0,08534149	0,34990847	4,98911988	-0,79170674	1,12609384
39	н	-5,33254031	0,55007699	0,73703079	5,45161323	-0,77111473	0,89718284	-6,08854017	0,48124847	1,03598645
40	C II	6,55168902	-0,77485116	0,53747887	-0,23044462	0,85220015	1,02700141	-0,05/88514	0,47119490	1,96969370
41	п ц	0,99233369 E 8071E2E2	-0,98812085	1,38104897	-7,00785949	1 82142421	1,76405550	-3,00430372	1,51515574	0,82590119
42	п Ц	5,89715255	-1,72212071	0,21572452	-5,76875445	0.80525462	0.04774491	-0,73880149	0,10050505	2 41560065
43	C C	4 60410252	0.25017620	-0,20050150	4 46994910	0,05555405	2 47400022	4,07281035	0.21552166	2,41300003
44	н	5 35597349	-0.25199307	3 05874694	-5 20414924	-0.08996329	3 27908308	-3 15688273	-0,59874418	2 52190779
46	н	3 78605911	0.40240688	2 57618018	-3 85992428	-1 05147049	2 66839339	-3 80330172	1 03682382	2,32130775
40	н	4 21553391	-1 26408032	2 18176730	-3 82437677	0 70860520	2,53661325	-3 41605163	-0.83558395	-2 52802708
48	C	3 21628250	1 45191463	-2 23198240	-3 52750971	-0.86393214	-2 42019045	-3 02936436	0 17247070	-2 65759940
40	н	2 71601694	0 51584440	-2 46637296	-3 10793361	0 13096635	-2 55728873	-2 58542710	-1 53601321	-2 67088117
50	н	2 44716268	2 21686287	-2 07349538	-2 69458605	-1 57459743	-2 41909108	-4 12519446	-1 03704119	-3 33665020
51	н	3,78210858	1.76646434	-3.11310334	-4.13840446	-1.10124659	-3.29265845	-1.37987536	3,41968047	0.10355116
52	C	1.60084733	-3.27983675	-0.21883844	-1.25272444	3,19416594	0.03895675	-0.63435619	4,19486849	-0.05372872
53	Ĥ	0.85258609	-4.05690695	-0.34822274	-1.12272589	3,30749842	1.11924979	-2.30960946	3,74200046	-0.37007019
54	н	2,41209614	-3.47139841	-0.92425344	-0.61292509	3,93994444	-0.43004352	-1.56969184	3,35634368	1.17993215
55	н	2,01450292	-3,39151590	0,78674588	-2,28275758	3,44186869	-0,20552856	2,64980065	-0,14995212	-0,10131778
56	С	-2,81211926	-0,04584675	0,57599218	2,83326178	-0,28440178	0,31915915	3,22468081	-0,97814464	0,30380086
57	н	-2,50837284	0,63225556	-0,22678609	2,40888840	-0,81883132	-0,53500490	1,74246561	-0,04194093	0,48930237
58	н	-3,46038260	0,51204165	1,24780740	3,48417484	-0,98468712	0,83770878	2,34950207	-0,43718740	-1,11201927
59	н	-1,91980983	-0,31387730	1,13607131	2,00754791	-0,02625785	0,98302880	7,08082753	-3,71183083	-1,22906901
60	н	-8,05239876	4,30927713	0,04782049	7,04337226	-3,92048379	-0,27641679			

Table S3. Cartesian coordinates (in Å) of the QM region of hWT carrying SBR

deprotonated. Ret_{gas} model.

• •	Ŧ		hWT	
Atom	Туре	х	У	Z
1	С	4,32167820	1,59391857	-0,66568565
2	Н	4,40148334	0,35528636	-0,10596901
3	Η	5,62794546	-0,11241742	0,71689087
4	С	6,46440684	1,10012441	1,17598535
5	Н	6,72164641	2,10172007	0,05990741
6	Н	5,39568465	2,63758744	-0,47055203
7	С	3,38599397	-0,66725968	-0,28960887
8	Η	2,03239783	-0,52315472	-0,28788981
9	Η	1,08697022	-1,58537819	-0,47010801
10	Ν	-0,25945279	-1,26927660	-0,34491214
11	Н	-1,33125019	-2,16191854	-0,52317098
12	С	-2,70330570	-1,99331077	-0,39641190
13	С	-3,48039798	-0,89451213	0,03476454
14	Η	-4,87231539	-1,05992982	0,02390771
15	Η	-5,81071027	-0,11994715	0,42116153
16	С	-7,12283764	-0,30846076	0,39613171
17	Н	-8,13163231	0,68168318	0,78362570
18	Н	-8,93291636	1,21308613	-0,40769428
19	С	-10,00201104	2,21546158	0,02909805
20	Н	6,49936148	-1,06268838	-0,13418113
21	Н	5,16833764	-0,86073176	1,98669574
22	С	3,19883758	2,06514688	-1,55257746
23	C	1,58645234	-2,96884237	-0,78153149
24	C	-2,84478326	0,38753751	0,49423012
25	н	-9,558/629/	3,07839579	0,53196680
20	с ц	-10,72069979	1,76013145	0,71447781
27	п С	-9,40346014	1,57265211	-0,92612575
20	c	-8,24497504	1,07852815	-1,11958576
30	н	-7,01270040	0.21664386	1,29307979
31	C	5 93582412	1 60588195	1 99172349
32	н	7.40572146	0.73524156	1.59617860
33	C	7.33893839	2,92754180	0.42063971
34	Н	7.28126601	1.63138638	-0.75305364
35	С	4,99431349	3,39048996	0,22371127
36	С	5,54657980	3,17188493	-1,41311053
37	Н	3,77164163	-1,67880590	-0,36778329
38	С	1,61152599	0,45681764	-0,09604014
39	Η	-0,47311532	-0,23834619	-0,10283450
40	С	-1,05841431	-3,16488333	-0,83143548
41	Η	-3,28269655	-2,87145333	-0,66201834
42	Η	-5,25169577	-2,01465023	-0,32839085
43	Н	-5,50666936	0,85167399	0,79128571
44	С	7,34246382	-1,42765558	0,45766464
45	Н	5,94024714	-1,93822364	-0,47216566
46	Н	6,89565502	-0,56537249	-1,02036455
47	Н	6,03413837	-1,10277542	2,60751277
48	C	4,48979476	-0,24623922	2,58320250
49	H	4,66072718	-1,80034802	1,75910904
50	п	2,59556852	1,25659880	-1,95786591
51	п	2,53515129	2,74544459	-1,00812525
52	ч	0 700442442	-3 7004032789	-2,30013090
54	н	2 16318396	-2 96909985	-0,88372092
55	Н	2,25093788	-3.32056983	0.01155227
56	c	-2.33379389	0.87722774	-0.33845216
57	H	-3,55799390	1,09849255	0,90273689
58	Н	-2,10021390	0,18829240	1,26669391
59	Н	-10,55659912	2,58572469	-0,83372722

Table S4a. Cartesian coordinates (in Å) of the QM region of bWT snapshots. Rho3

model.

	_		bWT1			bWT2			bWT3	
Atom	Туре	х	у	z	х	y	z	х	У	Z
1	С	10,23259100	-1,66589400	-11,21390200	10,29358900	-2,03116400	-11,55616900	10,31304300	-2,49447200	-12,13597200
2	Η	10,71681500	-1,11466900	-10,40747000	10,80519600	-1,48767400	-10,76018600	10,83746800	-1,93394100	-11,36099300
3	Н	10,26518200	-1,04706700	-12,12044600	10,30512900	-1,40714500	-12,45943300	10,31630100	-1,89619600	-13,05653100
4	С	8,75215600	-1,85925500	-10,88879900	8,81890200	-2,21662500	-11,18731100	8,84482200	-2,66500700	-11,74637200
5	0	8,00386000	-2,42559400	-11,/1884500	8,03222500	-2,71860500	-12,02240500	8,05411200	-3,21565000	-12,54720000
7	c	4,30233300	0,18290100	-6,92329500	4,24791400	-0,23168300	-7,33525100	4,37194900	-0,63034600	-7,92281500
8	Н	4,85821800	-0,69404200	-6,57964300	4,77125000	-1,12491100	-6,98261700	4,93320500	-1,50277400	-7,57724500
9	Η	3,38500900	-0,19058200	-7,38285200	3,33286500	-0,57636600	-7,82352300	3,44739300	-1,00606200	-8,36724500
10	C	5,10577700	0,91775500	-7,99508600	5,10597500	0,50863000	-8,36044100	5,16084700	0,10330300	-9,00400000
11	н н	4,67432800	1,89799000	-8,22423600	4,68621600	1,49151800	-8,59854300	4,70386300	1,06637500	-9,25599100
12	C	5.10863300	0.13312300	-9.31965800	5.20263500	-0.24780500	-9.69321700	5.20121200	-0.71046700	-10.30645400
14	Н	4,08073600	-0,00624500	-9,65853700	4,20407200	-0,38227700	-10,11413100	4,18250000	-0,88527700	-10,65822100
15	Н	5,63514900	0,69053600	-10,09576400	5,78801900	0,32737800	-10,41243100	5,73039900	-0,16257800	-11,08783300
16	Ν	5,74281200	-1,18429100	-9,24313200	5,83060500	-1,56257300	-9,58092400	5,86466300	-2,00414700	-10,16142800
17	Н	6,77774900	-1,24642600	-9,48479800	6,87368600	-1,63151700	-9,76623400	6,90913100	-2,04959400	-10,35447400
18	c	-0.28625600	-12,38394500	-6,69562300	-0 18717400	-13,14273900	-8,16653600	-0 10789700	-13,23760500	-7,98879300
20	Н	-0,82137000	-11,49909000	-5,55545200	-1,02869000	-14,28469400	-7,67940600	-1,02876200	-14,07180500	-7,35299700
21	Н	-1,02530400	-13,21817700	-5,85091100	0,35742400	-14,66244900	-6,67334300	0,33149600	-14,57234300	-6,36682200
22	С	0,30344600	-12,73504700	-4,21022700	-0,66577600	-12,89553000	-6,04623900	-0,39248300	-12,63069800	-5,85166000
23	H	-0,49267600	-12,79451900	-3,46266700	-1,18765000	-12,03518900	-6,47865800	-0,79010300	-11,73169500	-6,33535300
24	Н	0,80608400	-13,70555800	-4,20288600	-1,37999800	-13,39771700	-5,39133700	-1,15101800	-12,96648800	-5,14430100
26	н	0.75782800	-10.75368300	-3.46169000	0.26443300	-11.61209400	-4.56459700	0,78508500	-11.41814700	-4.48772200
27	Н	1,91377400	-11,97362900	-2,98946400	0,93205500	-13,22503900	-4,62503900	1,19322300	-13,11766200	-4,46352900
28	С	2,20008800	-11,19178700	-4,95386600	1,65879400	-11,90452200	-6,13833500	2,04290300	-12,01274800	-6,08838100
29	С	1,95944000	-11,47996900	-6,25498600	1,70670400	-12,15025600	-7,47108300	1,98027000	-12,33892100	-7,40313200
30	С	2,82462800	-11,00675300	-7,34463500	2,68076800	-11,51779100	-8,36372500	2,96447700	-11,86171300	-8,37991700
32	С	3 32577300	-11,72348600	-8,13501700	3,00402400	-10 25156200	-9,20779200	3,22402700	-12,54163500	-9,18471100
33	Ĥ	3,05579500	-9,03022000	-6,71300500	2,79494300	-9,61210200	-7,48630800	3,17057000	-9,91545300	-7,63998200
34	С	4,20339300	-9,26186300	-8,50753700	4,10442700	-9,64539200	-9,18763400	4,42127500	-10,08464600	-9,37236900
35	С	4,58400100	-7,94863000	-8,43037400	4,48296100	-8,34712100	-8,96290400	4,79356600	-8,77288700	-9,24188000
36	Н	4,16318400	-7,38065000	-7,61155000	4,00431600	-7,83641800	-8,13721200	4,32713400	-8,22199000	-8,43572400
37	н	6 15030200	-7,28250800	-9,27216200	5,50729400	-7,65058700	-9,66928600	5,77912700 6.45862400	-8,09233500	-10,01566300
39	C	5,81252200	-5,95001800	-9,39406300	5,83293900	-6,32161900	-9,71993100	6,05687000	-6,75654300	-10,12200700
40	Н	6,66930200	-5,71575300	-10,01667900	6,76434400	-6,09930900	-10,22990800	6,95624500	-6,51228600	-10,67634600
41	С	5,11261300	-4,78327900	-8,92303600	5,11575600	-5,14429600	-9,32160200	5,30032400	-5,59895000	-9,73083000
42	С	5,71103400	-3,56613900	-9,16428900	5,77043100	-3,94168700	-9,48496200	5,88889700	-4,37607300	-9,96904000
43	н	5,70848900	-3,56545300	-9,58789700	5 16439100	-3,95921300	-9,80218500	6,91185500 5 23875500	-4,36443600	-10,32540100
45	н	4.04087400	-2,20487600	-8.79817900	4.09305800	-2,57083400	-9.25472100	4.16867600	-3.05108800	-9.75217400
46	С	1,30902300	-13,80066700	-7,02098300	1,53248600	-14,25720700	-8,88841300	1,47098000	-14,50048500	-8,63848100
47	Н	1,78893200	-14,26362600	-6,15789000	2,09777000	-13,88837100	-9,74531900	2,07013000	-14,27527800	-9,52309000
48	Н	0,48902100	-14,44810100	-7,34399500	2,22964600	-14,75098500	-8,20777800	2,09590700	-15,04140300	-7,92403600
49	Н	2,04014600	-13,77352900	-7,83221800	0,83556400	-15,01169300	-9,26358500	0,66839500	-15,17188400	-8,95534400
51	н	0,03922200	-11,81790900	-8.81265800	0,11481200	-12,39639000	-9,21287000	-0.46238300	-12,469655500	-8,63256500
52	н	-0,74100100	-12,45839500	-8,23845800	-0,76388400	-13,09987600	-9,74184300	0,72070900	-12,08731000	-9,85347500
53	Н	-0,28468200	-10,81069800	-7,77315500	-0,74331100	-11,63471700	-8,74420300	-0,66902900	-13,12917600	-9,53304800
54	С	3,38459600	-10,40679900	-4,45748500	2,69802400	-11,13647800	-5,36396400	3,22369700	-11,36696800	-5,41022000
55	H	3,79496700	-10,89391100	-3,56971200	2,36062500	-10,11574700	-5,14887200	3,02512900	-10,31534900	-5,17432300
50 57	H H	4,18410000	-10,31313800	-5,18509500	2,84889800	-11,62708800	-4,39685300	3,40230900	-11,87854700	-4,45823700
58	C	4.63708500	-10.19009100	-9.60824900	4,59237600	-10.44529200	-10.36052300	4.89266600	-10.97163300	-10.48931400
59	Н	3,77236300	-10,70382900	-10,03577700	4,95885800	-11,42404300	-10,05051800	5,35040500	-11,88381400	-10,10274500
60	Η	5,13478500	-9,65979700	-10,41689500	3,76771700	-10,58838400	-11,06512600	4,04121600	-11,26032800	-11,11286000
61	Η	5,31727800	-10,95584700	-9,22898800	5,40246300	-9,94841300	-10,88743600	5,62200200	-10,47942800	-11,12868200
62	C	3,77481000	-4,89162400	-8,24543200	3,70448800	-5,20780900	-8,80864200	3,92031600	-5,72071100	-9,15076600
03 64	н н	3,22397600	-3,95296400	-8,26669000	3,69402500	-5,21199100	-7,715/3200	3,98026600	-5,91082200	-8,07555100 -9,28007200
65	Н	3,90728000	-5,15869200	-7,19228600	3,19804900	-6,10477000	-9,15153000	3,37712200	-6,54768600	-9,60246300
66	0	4,33641000	-4,72087100	-12,50512100	4,30102000	-5,03480400	-12,57562700	4,30163700	-5,44195900	-13,00131400
67	Н	5,20804300	-5,11545600	-12,48658100	5,17550700	-5,42381600	-12,55370700	4,49559900	-4,50440400	-13,01963200
68	Н	4,49392200	-3,78545300	-12,37673200	4,45740100	-4,09124300	-12,56938000	5,16010700	-5,86431800	-13,00518000
69 70	U L	9,12677100	-2,77642600	-7,52352300	9,45774700	-3,0/327500	-/,81523000	9,46413900	-3,50745400	-8,36958000
70	Н	8,92329100	-2.13485900	-8,20498400	9,52015900	-2,45027500	-8,48432300	9,18669000	-4,34227300	-9,03993100
72	Н	10,84212200	-2,53882800	-11,44740700	10,89536000	-2,90280100	-11,81343800	10,90061400	-3,38113900	-12,37398200
73	Н	4.01208400	0.74071300	-6.03297600	3.95876800	0.33841900	-6.45238900	4.10729500	-0.05543400	-7.03540300

Table S4b. Cartesian coordinates (in Å) of the QM region of hWT snapshots. Rho₃ model.

			hWT1			hWT2			hWT3	
Atom	Туре	х	у	Z	х	у	Z	х	У	Z
1	С	8,46491100	-3,27409800	-10,23559000	8,41296700	-2,77126600	-11,02262400	8,68163100	-3,50864700	-10,40196000
2	Н	8,92718900	-2,59510400	-9,51736600	8,78940000	-2,19786700	-10,17485300	8,86642200	-3,01275200	-9,44881100
3	Н	8,48438500	-2,78363000	-11,21793800	8,43165600	-2,10951800	-11,89908400	8,82811500	-2,75275000	-11,18582600
4	0	6,99236800	-3,46916800	-9,86055300	6,93888900	-3,12495500	-10,79348000	6 82922600	-3,90740200	-10,50304700
6	õ	6.56760200	-2.74560200	-8.92042500	6.37819300	-2.46408800	-9.85434000	6.41745100	-3.13105200	-9.85930900
7	C	2,39895200	-1,59649300	-5,34354700	2,52805600	-1,28073200	-6,60776400	2,64731200	-1,94245700	-6,73242400
8	Η	2,66883400	-2,60211500	-5,00756200	3,08228900	-2,16752400	-6,28876700	3,19958300	-2,84861500	-6,46785600
9	Н	1,43070200	-1,68106000	-5,84551200	1,59345300	-1,63176600	-7,05020300	1,68260000	-2,26329700	-7,13567900
10	C U	3,45222400	-1,09873700	-6,33515600	3,32643700	-0,48754800	-7,65373900	3,40762000	-1,15727600	-7,80663700
12	н	4 45608300	-1.24441600	-5,92653800	4.37316100	-0.39033300	-7,75059800	4 46089900	-0,14728100	-7,92339900
13	C	3,35687500	-1,80832800	-7,69486100	3,26053100	-1,06633800	-9,07837900	3,29985900	-1,80001100	-9,20319400
14	Η	2,50467800	-1,43027600	-8,26307300	2,22303200	-1,09647600	-9,41745100	2,25574500	-1,84745800	-9,51771300
15	Η	4,25430800	-1,63843500	-8,28794400	3,80533300	-0,41662400	-9,76393200	3,83451800	-1,19299000	-9,93421100
16	N	3,17047000	-3,26943500	-7,58939900	3,82706800	-2,40689400	-9,23181500	3,85773800	-3,15032000	-9,29106300
17	н С	2,22435600	-3,57109300	-7,37275300	4,85589700	-2,47932300	-9,53831300	4,88266400	-3,22859100	-9,57798100
19	c	-2.65580000	-13.36468500	-3.45041000	-2,46947000	-12,95965500	-4.91023600	-2.09122900	-14.31999700	-4.71881400
20	Н	-3,09391200	-12,36105600	-3,51309000	-2,88723700	-11,94840700	-4,98746500	-3,10008500	-14,62856300	-5,00900200
21	Η	-3,48078500	-14,07565200	-3,55540700	-3,30152500	-13,65672600	-5,04961200	-1,61401700	-15,20245000	-4,27864300
22	С	-1,97639600	-13,52160300	-2,09595200	-1,85008000	-13,13076500	-3,53011300	-2,13186800	-13,22360400	-3,66402100
23	H	-2,70588600	-13,39687400	-1,28974600	-2,60917400	-12,98441900	-2,75489600	-2,58680400	-12,31784600	-4,07816100
24	С	-0.85196400	-12 50266800	-1,99365900	-0.70863100	-12 14090000	-3,33157900	-0.71096000	-12 92662000	-2,81548200
26	н	-1,26092300	-11,52845800	-1,63739900	-1,10562500	-11,15570300	-3,04533800	-0,68273000	-12,01650900	-2,59349600
27	Н	-0,18147900	-12,80366600	-1,13259100	-0,08158300	-12,45543300	-2,49166400	-0,34486000	-13,73323000	-2,55426700
28	С	-0,03341400	-12,27493600	-3,19411400	0,16677800	-11,93425100	-4,54592900	0,25531500	-12,74699500	-4,34953300
29	С	-0,41751000	-12,69741800	-4,42052800	-0,18596300	-12,32284900	-5,79356600	-0,03863300	-13,10789300	-5,61982900
30	C U	0,34885700	-12,40495000	-5,63772100	0,62866600	-12,01743500	-6,97717400	0,81976800	-12,75531400	-6,75891600
32	C	0.88985300	-11.20371800	-5.93167700	1.22044100	-10.82466300	-7.20633100	1.39426100	-11.54596900	-6.93567800
33	н	0,74964800	-10,41130700	-5,20937000	1,08115800	-10,05526700	-6,45809000	1,21553900	-10,79573900	-6,17519100
34	С	1,66434000	-10,82973800	-7,09115100	2,01996700	-10,40309100	-8,33324200	2,23277700	-11,10651800	-8,02842500
35	С	2,13297100	-9,54258600	-7,14263500	2,44181100	-9,10025400	-8,33880400	2,65127900	-9,80446100	-8,02700100
36	Н	1,85224800	-8,89006600	-6,32465200	2,12408300	-8,49463200	-7,50142600	2,29236100	-9,17973000	-7,21924100
38	н	3,04804700	-9,80718000	-8,11519500	3,29303800	-9,18095600	-9,97652600	4 20627500	-9,22898500	-9,47642700
39	C	3,57140300	-7,79971700	-8,31120800	3,61704500	-7,17934200	-9,50568600	3,86460700	-7,92056800	-9,21581200
40	Н	4,38490400	-7,76339200	-9,02807700	4,38269000	-6,99829800	-10,25170700	4,71701900	-7,74815800	-9,86396800
41	С	3,23093100	-6,49893500	-7,80132400	3,05117400	-5,96618800	-8,97104100	3,16979300	-6,71072400	-8,85188700
42	С	4,16154100	-5,51130800	-8,03376100	3,66884100	-4,78758200	-9,31483300	3,77351100	-5,52497400	-9,19203400
43	н С	5,09851200	-5,82803000	-8,47665300	4,59382700	-4,81937200	-9,88361600	4,76373500	-5,55481800	-9,63853700
45	н	5.05485500	-3.60230100	-8.19121600	2.12253400	-3.37351500	-8.70270200	2.15547800	-4.11834100	-8.74880300
46	С	-1,29412600	-15,03665000	-4,78434700	-1,07094500	-14,64908900	-6,18661600	-0,93591300	-15,20747800	-6,72692100
47	Н	-2,18855700	-15,64614600	-4,94689100	-0,61493000	-15,03145800	-5,27290300	-0,20367900	-15,78605000	-6,16001900
48	Н	-0,62792900	-15,19206100	-5,63572400	-1,95618900	-15,25352200	-6,40954300	-1,82989700	-15,82508000	-6,85490100
49	н	-0,78136100	-15,41046900	-3,89734800	-0,35458100	-14,80032300	-6,99706600	-0,52467000	-15,02421100	-7,72106300
51	н	-1.83888300	-13,26014500	-6.81264700	-2.43772800	-11.66733100	-7.30323500	-1.64618100	-12.71183200	-7.77481400
52	н	-3,34833000	-13,69340900	-6,00969600	-1,53402100	-12,86474400	-8,23911100	-3,04726500	-13,66049800	-7,26212000
53	Η	-2,70288000	-12,05065500	-5,85978200	-3,06888500	-13,31102200	-7,49738300	-2,60018600	-12,17959600	-6,39181500
54	С	1,24714500	-11,53547400	-2,92265800	1,46620600	-11,25812800	-4,20986700	1,57034800	-12,16129000	-3,91543800
55	H	1,98945300	-11,66471800	-3,70448400	2,23578000	-11,42122800	-4,95873000	1,84932700	-12,59044300	-2,94849500
50	л н	1,07247800	-10,46069400	-2,80590200	1,34554800	-11 64810100	-4,08562700	2,37536000	-12,36765800	-4,61507500
58	C	1,95306100	-11,85887000	-8,14771300	2,31915000	-11,36443200	-9,44837400	2,57800900	-12,05174400	-9,14374500
59	Н	1,08561300	-12,49937400	-8,31665400	3,30967200	-11,19426700	-9,86759000	2,48024800	-13,09129500	-8,83894900
60	Н	2,21861900	-11,40491100	-9,10034500	2,29262000	-12,39756100	-9,10624800	1,91915400	-11,88255100	-10,00208000
61	Н	2,78470300	-12,49625300	-7,83667900	1,58566900	-11,25950300	-10,25496000	3,60827300	-11,91322000	-9,46928900
62	С Н	2,03750400	-6,19/81000	-7,15089300	1,83825300	-5,98/4/900	-8,08036500	1,82894600	-b,/b069600	-8,16668/00
64	Н	1,37216800	-5,44658100	-7,73912500	1,15163100	-6,78460900	-8,35517700	1,23071800	-7,59184600	-8,53850400
65	Н	1,26505600	-7,06977400	-7,08783100	2,14588700	-6,16123400	-7,04525600	1,95515000	-6,91036500	-7,09066000
66	0	3,40146300	-4,69970000	-10,97133200	2,46893700	-4,67956100	-12,50177700	2,46036400	-5,54455400	-12,33885800
67	H	4,30075900	-4,49400000	-10,71485600	1,72505900	-5,22260400	-12,76250400	1,82024200	-6,12642000	-12,74774300
68	H	3,44310500	-5,60407700	-11,28421200	3,20437000	-5,28897800	-12,44756100	3,24080900	-6,08653500	-12,22764200
70	Н	7,45763900	-3,79445100	-6,85257000	7,08359900	-2,91641600	-7,45480600	7,70087300	-1,95385300	-7,45024000
71	Н	7,18393200	-3,23692300	-7,25122300	7,56407300	-4,31492600	-7,83223100	6,63702000	-2,34459500	-8,28727000
72	Н	9,10489100	-4,15047400	-10,33784900	9,11643200	-3,56847400	-11,26275800	9,45425500	-4,25619700	-10,58164500
73	H	2,24258200	-0,99034800	-4,45124500	2,26772600	-0.70897700	-5,71704000	2,44913500	-1,40253300	-5.80653300

Table S4c. Cartesian coordinates (in Å) of the QM region of hS186W snapshots.

Rho3 model.

	_		hS186W1			hS186W2			hS186W3	
Atom	Туре	х	v	z	х	v	z	х	v	z
1	С	10,59271300	-5,37577300	-9,75121700	10,08436400	-4,26874700	-10,27285400	10,04178000	-4,27936300	-9,36561200
2	н	10,78611800	-4,33124400	-10,02220400	10,34779000	-3,26193700	-10,61539300	10,22555500	-3,22815600	-9,61620400
3	Н	10,98808700	-6,00681700	-10,54209800	10,39208700	-4,97943600	-11,03444900	10,49752000	-4,89661400	-10,13489200
4	С	9,09563700	-5,55371700	-9,70896400	8,58776000	-4,31597400	-10,14660400	8,54958700	-4,49181100	-9,40448000
5	0	8,49500500	-6,22746100	-10,51409700	7,88339300	-5,04896400	-10,79756600	8,00086200	-5,22076900	-10,19950500
6	O C	8,47921500	-4,86279800	-8,73298700	8,07143000	-3,42882200	-9,25835600	7,87381400	-3,75892700	-8,49985400
8	н	1 88104600	-5,08773500	-8,71608100	1 57799600	-3,56510300	-9,19289500	1 14972100	-4,03278400	-8,48809400
9	н	2.88013300	-4.67006600	-6.09830700	2.59082600	-4.17897100	-6,73361900	2.23293100	-2,74619600	-5.78465600
10	С	1,15805500	-5,04448800	-6,07922000	0,87804000	-4,58921400	-6,63242000	0,68949200	-3,58972900	-5,69770400
11	Н	1,72757200	-3,67435300	-7,64128200	1,33840400	-3,18392300	-8,20401700	0,68253700	-1,98999600	-7,15568600
12	Н	0,71669900	-3,28303700	-7,79664400	0,31019900	-2,81645800	-8,29449800	-0,40468400	-2,04812200	-7,20210100
13	С	2,41771400	-2,84162100	-7,80332200	2,00160300	-2,33228300	-8,37953400	0,91789500	-0,91833400	-7,17386500
14	H	2,01757800	-4,71358900	-8,73716000	1,57680900	-4,18003700	-9,34811100	1,21320200	-2,49897800	-8,51166500
15	H N	2,02971100	-4,21366600	-9,/101/000	1,54438700	-3,62686200	-10,29291700	2,21577600	-2,02405100	-9,28478500
17	н	0 98249000	-5 73704700	-8 79242100	0 53799800	-5 19134900	-9 42732500	1 33855200	-3 90159700	-8.89476700
18	C	-1,11120400	-15,31337600	-6,92777700	-1,31669100	-14,99774600	-7,36260900	-1,36801200	-14,72015600	-6,89430000
19	С	-2,18840500	-15,89367800	-5,98828300	-2,38271900	-15,59294000	-6,42206700	-2,46663600	-15,31233100	-5,99175300
20	Н	-2,38265500	-15,17079300	-5,18693800	-2,67940600	-14,82791800	-5,69504900	-2,80671700	-14,54069700	-5,29107800
21	Н	-3,12029100	-16,00232600	-6,55176900	-3,27588300	-15,83188400	-7,01000900	-3,32986500	-15,57260400	-6,61383200
22	С	-1,79041100	-17,22160700	-5,36058700	-1,88980200	-16,81533600	-5,66429600	-1,99199000	-16,51733500	-5,19574800
23	н	-2,60027700	-17,60224600	-4,/311/600	-2,68935400	-17,22416500	-5,04120000	-2,81/21900	-16,92995000	-4,61138000
24	с	-1,63266200	-17,97219500	-6,14041500	-1,60684100	-17,60754700	-6,36400300	-1,66640000	-17,31127200	-5,87452200
26	н	-0.76119400	-16.56390300	-3.57688200	-1.03405200	-15.91775800	-3.89742200	-1.23324200	-15.58019000	-3.40345500
27	Н	-0,09953400	-18,01918800	-4,27242000	-0,18705600	-17,34217100	-4,44246300	-0,33459900	-16,99272300	-3,88127900
28	С	0,54707800	-16,21623600	-5,21897000	0,32296400	-15,55557400	-5,49218900	0,19125000	-15,21621500	-4,94120000
29	С	0,29231900	-15,44213000	-6,29171100	0,04734000	-14,89744500	-6,63778800	-0,04123500	-14,58090500	-6,10729500
30	С	1,36922400	-14,69689100	-6,99278700	1,05888000	-14,08334900	-7,33678700	1,00032500	-13,78081700	-6,78981000
31	Н	1,62058400	-15,06615100	-7,98453800	1,22347000	-14,34378500	-8,37886700	1,30054000	-14,16278600	-7,76294900
32	ч	1,98398100	-13,59268800	-6,54199000	1,72136000	-13,02743200	-6,83404900	1,52683400	-12,61061000	-6,38712500
34	C	3.01379500	-12.83304100	-7.24841500	2,69409600	-12,20911700	-7.56328700	2.47445800	-11.82337000	-7.17011800
35	C	3,30029700	-11,56270300	-6,86023100	2,93067600	-10,92623300	-7,18348200	2,54141200	-10,46841900	-7,00826300
36	Н	2,73710900	-11,18440700	-6,01450400	2,37527300	-10,55489100	-6,32844900	1,93739100	-10,03136400	-6,22075600
37	С	4,25377000	-10,66002700	-7,49743400	3,85946600	-10,00049800	-7,83441300	3,23401900	-9,58132400	-7,91360900
38	Н	5,16074500	-11,11097000	-7,89093600	4,81465900	-10,42184800	-8,13810800	3,98531800	-10,05173900	-8,53700800
39	C u	4,11292200	-9,34251200	-7,75860200	3,66821000	-8,/1206100	-8,18188400	3,01091200	-8,28145100	-8,23691000
40	п С	2 94459200	-8,90347100	-8,37049700	4,47589200	-8,23143800	-8,74366300	2 14855500	-7,93703200	-7,68097500
42	c	2,58368200	-7.64326500	-8.52544400	2,14964500	-7.08456000	-9.11287100	1.92187200	-6.16229000	-8.47254500
43	н	3,21711200	-7,57535300	-9,40654000	2,84830700	-7,02845600	-9,94515300	2,29563100	-6,18729500	-9,49204100
44	С	1,27143400	-6,96424800	-8,62527000	0,83222100	-6,41869500	-9,28614700	1,42958500	-4,86674800	-8,05956000
45	Н	0,42157200	-7,65506700	-8,63008800	-0,01232500	-7,11381700	-9,32477600	1,26051200	-4,72130700	-6,99867600
46	С	-1,15751000	-16,03037800	-8,29330700	-1,19330200	-15,87299800	-8,62813900	-1,16337400	-15,62603800	-8,12793400
47	H	-0,38652000	-15,65668600	-8,96765700	-0,43610800	-15,48654700	-9,31129600	-0,39237600	-15,23078100	-8,78988400
48	п	-1,02941200	-17,10826000	-8,19057300	-0,93106000	-15,90200900	-8,37906900	-0,87436200	-15,63634000	-7,83678600
50	C	-1.44708800	-13.83073400	-7.16780500	-1.79606000	-13.59956300	-7.79321700	-1.85610900	-13.34462400	-7.38161700
51	н	-2,46711100	-13,72773400	-7,54662400	-1,11646600	-13,13912200	-8,51014900	-1,15833100	-12,88963400	-8,08412100
52	Н	-1,37185300	-13,25215500	-6,24390500	-2,77547000	-13,66532000	-8,27412300	-2,81658200	-13,44423700	-7,89491600
53	Н	-0,78091600	-13,38316000	-7,90512900	-1,88778900	-12,93069100	-6,93427700	-1,99366900	-12,65510400	-6,54519700
54	С	1,90435500	-16,37588800	-4,58308300	1,65805200	-15,53251600	-4,79141200	1,48788500	-15,15679800	-4,17604100
55 56	H	2,21992000	-17,42337800	-4,63308500	1,94792000	-16,54607000	-4,50287600	1,92558800	-16,15872100	-4,11055800
57	н	1 86270800	-16 12372700	-3,51831900	2,43239400	-13,12401900	-3,41109400	2,22856500	-14,49401200	-3 14333200
58	C	3,68451800	-13,49190300	-8,41780700	3,39150500	-12,84078200	-8,73573300	3,26731300	-12,55180500	-8,22255000
59	Н	4,15504300	-14,42876800	-8,10855900	4,06279000	-12,14589800	-9,23843400	3,56967000	-13,53161400	-7,85130400
60	Н	2,94714000	-13,75596800	-9,18161700	3,97488500	-13,70601700	-8,40835400	2,66007700	-12,72924200	-9,11616500
61	Н	4,44796900	-12,86328900	-8,87247900	2,67344200	-13,21653900	-9,46796700	4,16759800	-12,01597100	-8,51692600
62	С	2,19594800	-8,46305300	-6,21700300	1,63320400	-7,87777400	-6,80873700	1,61904800	-7,36659700	-6,27500000
63	H U	2,34026600	-9,36123300	-5,62450000	2,21906000	-/,44112400	-5,99382700	1,25663900	-6,41751400	-5,88440700
65	н	2,55575000	-7,02341400	-5,61089200	1 34488300	-7,27897600	-6,91704600	2 38040100	-0,00242300	-0,24012500
66	0	1,46648000	-4.25991800	-12,58915700	2,17655400	-2.16718000	-14,26178400	2,20463500	-2,83638100	-13.82777500
67	Н	1,42204400	-4,48179400	-13,51895600	1,78163900	-2,98683400	-14,56085700	1,82558900	-3,03272000	-12,97053000
68	Н	0,80401900	-4,81546700	-12,17738300	1,48163500	-1,73350900	-13,76626400	1,86189000	-3,52007300	-14,40324800
69	0	2,02688800	-7,53719400	-0,32606900	8,13145700	-4,42746100	-6,29531900	3,49843300	-7,41523100	-1,86300400
70	H	1,60082400	-6,78830000	-0,74400200	8,12410500	-3,85608300	-7,06272700	4,05707500	-8,18424300	-1,97695500
71	H U	2,82407700	-7,67603900	-0,83741000	8,43869700	-5,2/105800	-6,62753300	3,32462900	-7,38198000	-0,92225000
72	н	1 73645400	-3,55183100	-8,82146300 -5.43238900	1 45589400	-4,45399600	-9,35416600	10,52651100	-4,44747700	-8,40392600

Table S5. Cartesian coordinates (in Å) of the QM region of hWT, hM207R and hS186W. **Rho₄** model.

	<i></i>		hWT			hM207R			hS186W	
Atom	Туре	х	У	Z	х	у	Z	х	У	Z
1	С	-8,05422754	3,35775057	0,57047248	-6,72966180	-2,99035866	0,18946164	-6,92650986	-2,48782497	1,04004832
2	н	-7,52272154	3,34324186	1,52387157	-6,02988347	-2,50256939	0,87466969	-6,60168087	-1,65881087	1,67182885
3	н	-9,11387783	3,21426717	0,80548180	-6,26837154	-2,97947272	-0,80197921	-6,05982146	-2,78926955	0,44974702
4	С	-7,55026739	2,19156492	-0,28441717	-8,06286366	-2,23217659	0,17043289	-8,03660880	-2,04102802	0,08095976
5	н	-8,01850305	2,17586059	-1,27094110	-8,84488370	-2,82023046	-0,32245029	-8,59440961	-2,88640035	-0,32535619
6	н	-6,47103087	2,27974416	-0,44324351	-8,41714841	-2,04704345	1,18858691	-8,77006778	-1,41988067	0,58244545
7	С	-7,82764908	0,85178905	0,42827916	-8,02858784	-0,90686750	-0,60700166	-7,52444756	-1,28173966	-1,15136540
8	н	-7,62571716	0,96228382	1,49600757	-7,75865628	-1,08615906	-1,64945826	-6,84813744	-1,93936008	-1,70616925
9	н	-8,87128044	0,55950255	0,32169034	-9,01630856	-0,45040773	-0,60787472	-8,37435729	-1,05872029	-1,79938373
10	N	-6,99870843	-0,25480370	-0,06918727	-7,09375453	0,10107840	-0,07542881	-6,85275843	-0,03082708	-0,82494618
11	н	-7,41319603	-0,97726946	-0,71589281	-7,48395222	0,89696502	0,49585462	4,84996687	-0,43255158	-1,17516951
12	С	5,31623313	0,27419995	0,89386571	5,02669726	-0,46604560	-1,16784386	5,35491133	-1,88847686	-1,21780524
13	С	5,90598683	1,68241496	1,10874583	5,89468964	-1,73291114	-1,02013232	4,49789794	-2,55217201	-1,38425910
14	н	5,18192526	2,27876539	1,67666399	5,24702640	-2,60344756	-1,14855318	6,01744849	-2,01273844	-2,08007111
15	н	6,79843844	1,60193027	1,73618136	6,61517663	-1,76220436	-1,84306209	6,06656244	-2,29869947	0,06399832
16	С	6,21589245	2,40506367	-0,19254326	6,59836716	-1,83376954	0,32561370	6,41287947	-3,33323828	-0,00682779
17	н	6,63980502	3,39221541	0,01228239	7,22339052	-2,72940227	0,36565632	6,96090088	-1,68497613	0,20357489
18	н	6,96999691	1,85458944	-0,76186506	7,27278155	-0,98669126	0,48012651	5,142/1/52	-2,13921184	1,26648591
19	C	4,94379536	2,54882402	-1,02169415	5,55856456	-1,87656072	1,43/1256/	4,50520612	-3,02/9998/	1,37688435
20	н	4,34527218	3,39259935	-0,64890640	5,09295831	-2,8/1//161	1,48822034	5,73731608	-2,09450415	2,18501902
21	н	5,19522870	2,80629636	-2,05522070	6,03522356	-1,72970796	2,41034700	4,23311344	-0,93546226	1,231///89
22	C	4,04742098	1,33191258	-1,03357515	4,44466482	-0,86/31660	1,29066749	4,04879119	-0,184/1513	0,12381715
23	C	4,16401308	0,32326234	-0,135555459	4,19468314	-0,21318167	0,12062777	3,11934735	0,95279371	0,08619553
24	L L	3,27000209	1 70052522	-0,11517525	3,13413304	1 60060942	0,01945096	3,47940182	1,65190095	-0,40690411
25	п С	1 02002000	-1,79055522	0,12000018	1 00717592	0,82052720	-0,71413136	1,03120271	0,93089385	0,54005272
20	L L	1,52505055	0 15140929	-0,28210180	1,50717585	0,82952720	1 12/55277	0.97/12707	2 00072367	0,30484720
28	C	1,43030003	-1 93769883	-0,43349514	0.90203879	1 87263494	0.38956421	-0.42146279	1 70329161	0,47505020
20	c	-0 31679779	-1 66388298	-0.35862600	-0 41199751	1 53629829	0 54785127	-0.61844881	0.67990071	1 04821069
30	н	-0 58462039	-0.61612248	-0 38130718	-0 63461545	0 49543443	0 75319018	-1 55594515	2 59323303	0 70430870
31	C	-1 36860116	-2 61286255	-0 50974552	-1 51358908	2 46365479	0 52252782	-1.35230316	3 64366575	0 89745498
32	н	-1.06014586	-3.61451744	-0.79245229	-1.25205299	3,48880830	0.77069270	-2.85956472	2,29706679	0.45990877
33	С	-2.72476845	-2.42899218	-0.44532266	-2.83995700	2.24013367	0.32509701	-3.56422966	3.11924032	0.54878386
34	н	-3,33285996	-3,27412710	-0,74662257	-3,49174734	3,09020536	0,49491034	-3,47485797	1,05553614	0,02004045
35	С	-3,49093656	-1,31216850	0,02703437	-3,56493410	1,05767591	-0,10706224	-4,82033953	1,06133958	-0,20039961
36	С	-4,85413045	-1,33953299	-0,20240466	-4,91863160	1,08543247	0,09177462	-5,37740289	1,97991331	-0,04630954
37	н	-5,29208492	-2,17262838	-0,74621871	-5,34845854	1,93739403	0,60183889	-5,59375246	-0,08316669	-0,61765354
38	С	-5,73116408	-0,33462215	0,23939303	-5,82505584	0,09575495	-0,36070620	-5,06648000	-1,03493686	-0,72544321
39	н	-5,37520215	0,45786800	0,89013243	-5,49286059	-0,71133122	-1,00409911	6,03934765	0,54878517	-1,23025481
40	С	6,39769907	-0,70278235	0,38257839	5,94375045	0,73369982	-1,49378916	6,57825429	0,44574110	-2,17732424
41	н	7,17677959	-0,84616129	1,13739312	6,60335984	0,48769449	-2,32904434	5,69212519	1,58121694	-1,15974576
42	н	5,97464604	-1,68519438	0,16527371	5,37050449	1,60476946	-1,83107871	6,74354604	0,38408273	-0,41478108
43	н	6,87020345	-0,34342795	-0,53234225	6,58222339	1,00871324	-0,65079427	3,97791452	-0,21093465	-2,42690436
44	С	4,82326255	-0,21619043	2,26871986	4,08748479	-0,68191379	-2,37290774	4,55048831	-0,45498771	-3,32587513
45	н	5,67130900	-0,28101755	2,95744484	4,67500785	-0,90587251	-3,26630898	3,09312636	-0,84970958	-2,41093481
46	н	4,10826027	0,49153790	2,69331890	3,41489955	-1,52451045	-2,20524998	3,64262353	0,82359733	-2,52364359
47	н	4,34915170	-1,19551388	2,22912858	3,47758222	0,19489407	-2,59535014	3,58124956	-0,67359435	2,56439860
48	C	3,04170055	1,37030055	-2,152/2/3/	3,64431346	-0,68960957	2,55/21560	3,13344814	0,31401487	2,64219442
49	н	2,59404723	0,40441683	-2,37044444	3,18438238	0,29334219	2,65199037	2,80508662	-1,42094368	2,76941513
50		2,23189320	2,07235751	-1,92554844	2,83874558	-1,43014946	2,59366600	4,33568491	-0,76791601	3,351/9624
51	П	3,33103/5U 1 59339653	1,72911013	-3,00093113	4,2/808//8	2 28861220	5,42959939 0.07122609	1,31348612	3,3399382/ 1 10232871	0,01559972
52	μ	1,20332023	-3,32839096	-0,17743250	1,51/08494	3,20001/29	-0.86007367	0,52707481	3 60035003	0,130903/8
55	н	2 10780225	-4,07012231	-0,05018479	1 00078712	3,050/92/5	0,80007207	2,10/3044/	3,05023863	-1 04424270
55	н	2,10780225	-3 41076352	0.64791965	2 39741433	3 38644506	-0.00956654	-2 63654653	-0 17413278	-0 23136575
56	C	-2 82492621	-0.18266300	0 77264514	-2 86253804	-0 10038339	-0 75925444	-3 14945182	-0 9132/102	-0.83957122
57	н	-2.39749841	0.54364290	0.07543272	-2.27818686	-0.66658071	-0.02967855	-1.72123259	0.09413783	-0.75413166
58	н	-3,51526692	0.35740477	1.41719038	-3.54614253	-0.79886817	-1.23568270	-2.35018306	-0.65776734	0.70731909
59	н	-2,01404991	-0,55824453	1,39511046	-2,17720505	0,25834091	-1,52695465	-7,17347493	-3,31838585	1,70131861
60	н	-7,96115204	4,36281155	0,15899697	-6,80611802	-4,03255661	0,49941196			

Table S6. Cartesian coordinates (in Å) of the QM region of hWT, hM207R and hS186W. **Rho₅** model.

			hWT			hM207R			hS186W	
Atom	Type	х	у	Z	х	у	Z	х	У	Z
1	С	-8,22891689	3,30591851	0,66400805	-6,84126936	-2,85452063	0,41191869	-6,87937843	-2,50613259	1,08906249
2	н	-7,72182729	3,26071072	1,62887963	-6,19510954	-2,27039101	1,07465997	-6,56983392	-1,66271223	1,70899721
3	н	-9,29095684	3,12556572	0,85582696	-6,31433788	-2,95621910	-0,53827873	-6,00132102	-2,81103747	0,51758163
4	С	-7,65875195	2,21351582	-0,23954498	-8,16686122	-2,13248837	0,18101597	-7,97731988	-2,08454373	0,10499926
5	н	-8,13774997	2,21652366	-1,22088066	-8,90808683	-2,78877571	-0,28659007	-8,52334333	-2,94144434	-0,29382823
6	н	-6,58698106	2,36933699	-0,40016073	-8,61341464	-1,80059897	1,12356254	-8,72217041	-1,45963662	0,58532757
7	С	-7,83233458	0,82954138	0,40053873	-8,01716751	-0,93896108	-0,76879335	-7,44831700	-1,34431555	-1,13255727
8	н	-7,57972102	0,87791458	1,46055998	-7,64999322	-1,26341166	-1,74224351	-6,75450345	-2,00725013	-1,65881851
9	н	-8,86546896	0,48674026	0,32680608	-8,97217935	-0,44786956	-0,93713111	-8,28653942	-1,14235285	-1,80221052
10	N	-6,96608020	-0,18385215	-0,21143567	-7,08301176	0,08938256	-0,27841648	-6,79445993	-0,08119768	-0,81848024
11	н	-7,27582919	-0,61534878	-1,09307908	-7,49738654	0,8941/113	0,17475051	4,77154090	-0,58280000	-1,19959430
12	C	5,37403082	0,28240078	0,84987285	4,97739129	-0,52325757	-1,201/1919	5,42755995	-1,96/3295/	-1,02/44663
15	C	5,95500245	1,69450649	1,06380911	5,79116553	-1,82206178	-1,02633490	4,64212046	-2,73205011	-1,050/4/06
14	н	5,24964447	2,27455689	1,67012006	5,09524645	-2,66404902	-1,06354592	6,07615192	-2,16359420	-1,88618309
15	П	6,87074601	1,01229085	1,05515095	6,45921428	-1,93435921	-1,88504069	6,20112681	-2,09557472	0,27652708
17	U U	6,20969552	2,44094714	-0,23429088	0,00002480	-1,8/910035	0,28256907	0,07002702	-3,08073536	0,34691188
18	н	6 95717621	1 91644927	-0,023333364	7 28346093	-2,79808780	0,34133004	5 26519914	-1,30108507	1 45720602
10	п С	4 90985870	2 57295629	-0,83328233	5 58834538	-1,03810475	1 4/906963	1 66798439	-1,87723321	1,43720002
20	н	4 31557965	3 40868693	-0.62356602	5 09969041	-2 78869730	1,59590564	5 84436573	-1 72412479	2 37305670
21	н	5 12030080	2 83973588	-2.06122833	6 11853611	-1 61410021	2 38417767	4 30266435	-0 72561460	1 29628487
22	c	4.01166375	1.36112518	-1.00698917	4.48540953	-0.79737795	1.29713873	4.02976854	-0.16656258	0.09477332
23	c	4.16556133	0.34160429	-0.11529546	4,19868451	-0.19303469	0.10372000	3.04750954	0.91149701	-0.07086482
24	C	3,27947382	-0,80750152	-0,06341748	3,15226664	0,82199915	-0,03252515	3,31921455	1,69019834	-0,77786029
25	н	3,74401915	-1,75079997	0,20823843	3,35481742	1,58490552	-0,77931075	1,83501560	0,97019421	0,51457961
26	С	1,92737885	-0,79962464	-0,22863301	1,94824374	0,89479292	0,58848084	1,55066633	0,15359173	1,16770239
27	н	1,44541038	0,15584812	-0,38264253	1,64326483	0,07526300	1,22641968	0,80603228	1,97688500	0,33504673
28	С	1,04956987	-1,92931283	-0,21367090	0,94084804	1,91595811	0,39172175	-0,42779912	1,75049471	0,85043780
29	С	-0,31063027	-1,67025378	-0,29741242	-0,37752105	1,56554290	0,57788307	-0,57804807	0,81807147	1,38084160
30	н	-0,59606618	-0,62647048	-0,28337813	-0,57822313	0,53588404	0,84576534	-1,56987874	2,64212223	0,73668983
31	С	-1,32573691	-2,61706873	-0,51617417	-1,48005464	2,46185336	0,46639514	-1,36496927	3,70137469	0,88205132
32	н	-0,99964601	-3,60873419	-0,81384562	-1,22782652	3,51374714	0,57059275	-2,86390549	2,33225324	0,48421566
33	С	-2,69961072	-2,42237896	-0,53434109	-2,82089469	2,21655696	0,29777894	-3,57562134	3,15119183	0,51966393
34	н	-3,27798884	-3,22172260	-0,98826742	-3,45667913	3,09174849	0,37210877	-3,45202770	1,06376507	0,07896500
35	С	-3,46740730	-1,36828280	0,01228296	-3,53017744	1,01005235	-0,01687905	-4,78859479	1,04814057	-0,18111175
36	С	-4,82020109	-1,28057629	-0,33965400	-4,91354281	1,07093829	0,01048894	-5,35581379	1,96636789	-0,07316424
37	н	-5,18768850	-1,96109984	-1,10294512	-5,36800444	1,99215021	0,36030582	-5,53870840	-0,11548091	-0,58889664
38	C	-5,72446580	-0,37595080	0,20363861	-5,77857132	0,05472364	-0,41970641	-4,99725615	-1,06202367	-0,67081334
39	н	-5,44197278	0,24002170	1,05221996	-5,40097287	-0,82172611	-0,93357634	5,84683132	0,47246335	-1,54045019
40	L L	7 24045976	-0,67251927	0,25911474	5,93030108	0,02425540	-1,005555594	6,36196034 E 40207164	1 45906469	-2,46749019
41	п ц	6 00691314	-0,65160270	0,96955710	5 27606471	1 40070017	-2,45400625	5,40507164	0.56160456	-1,09107150
43	н	6 85929261	-1,05205558	-0.66708450	6 59336818	0.92332380	-1,38473073	3 80129339	-0.69085085	-0,74807823
44	C	4 96065416	-0 23388561	2 24108140	3 99677066	-0 74557469	-2 37113387	4 34727589	-1 00543347	-3 28636103
45	Ĥ	5.84181107	-0.27629000	2.88748517	4,54888740	-1.02131391	-3.27196666	3.03073545	-1.43840233	-2.19715778
46	н	4.24731221	0.45199644	2,70234373	3.30196339	-1.55810118	-2.15600286	3,30566335	0.25304442	-2.62604093
47	н	4,51632598	-1,22781388	2,21894677	3,41355650	0,14534524	-2,61083778	3,69425174	-0,28697202	2,60443246
48	С	2,97128306	1,40769354	-2,09234743	3,74514243	-0,53666123	2,58320721	3,29885978	0,72634117	2,57755523
49	н	2,50320583	0,44906712	-2,29830786	3,32776875	0,46670249	2,65710558	2,88216260	-0,96199256	2,90157486
50	н	2,18344737	2,12624204	-1,83973613	2,91465725	-1,24386446	2,67920316	4,45551012	-0,33296566	3,38774162
51	н	3,43823776	1,76170909	-3,01400468	4,40619405	-0,69265772	3,43577733	1,08910379	3,21576405	-0,46574252
52	С	1,60699295	-3,31957029	-0,13243701	1,33871727	3,31026071	-0,01693105	0,18592081	3,58731043	-0,95007691
53	н	0,84248449	-4,05381573	0,11454413	0,78670021	3,66033881	-0,89381692	1,48807293	4,00677950	0,17680733
54	Н	2,03803219	-3,60419283	-1,09553353	1,13517359	3,99738960	0,80976399	1,82968431	3,03242447	-1,24414181
55	н	2,39343509	-3,38670335	0,62154403	2,40265219	3,38692883	-0,22954353	-2,58756096	-0,15978064	-0,09898538
56	С	-2,86316866	-0,38399758	0,98059392	-2,81071290	-0,26395873	-0,35819859	-3,05800529	-0,91814244	-0,71857925
57	Н	-2,51551621	0,51318377	0,45962306	-2,42607023	-0,73587902	0,55082584	-1,64654991	0,11073332	-0,57291649
58	н	-3,58708977	-0,05637803	1,72570903	-3,44829526	-0,99216368	-0,85338388	-2,34553184	-0,62008938	0,86396782
59	н	-2,01493312	-0,81/94051	1,50518092	-1,96102783	-0,06915891	-1,008/0037	-7,12868875	-3,32483381	1,76403833
00	н	-8,13749559	4,32635308	0,291/5121	-6,91420390	-3,85518641	0,83786726			

Table S7. Cartesian coordinates (in Å) of the QM region of hS186W. Rho_6 model.

Atom	Туре	hS186W		
		х	v	Z
1	C	-6 92113326	-2 50162490	1 02895756
2	н	-6.59574540	-1.67582267	1.66491949
3	н	-6.05437543	-2.80254976	0.43827217
4	С	-8,02973722	-2,04896578	0,07071239
5	Н	-8,58482050	-2.89229146	-0.34377673
б	Н	-8,76578562	-1,43412548	0,57625957
7	С	-7,51870895	-1,27878413	-1,15574290
8	Н	-6,84432970	-1,93230159	-1,71742599
9	Н	-8,36721604	-1,04797543	-1,80137369
10	Ν	-6,84458857	-0,03201184	-0,82076029
11	Η	4,84992982	-0,42690564	-1,17046779
12	С	5,34063830	-1,88671579	-1,22857452
13	С	4,47785576	-2,54028888	-1,40529069
14	Η	6,00536928	-2,00766310	-2,08961567
15	Η	6,04400361	-2,31853365	0,05074508
16	С	6,37867404	-3,35612853	-0,03029813
17	Η	6,94513188	-1,71665471	0,19798358
18	Η	5,12131960	-2,16037087	1,25408708
19	С	4,47773039	-3,04543942	1,35985465
20	Η	5,71664832	-2,12534464	2,17275819
21	Η	4,21931658	-0,95092293	1,22778215
22	С	4,04343380	-0,18825476	0,12661868
23	С	3,12067223	0,95440677	0,09480128
24	С	3,48596566	1,85446371	-0,39270650
25	Η	1,85073388	0,93526236	0,54450489
26	С	1,47873193	0,00702688	0,96307308
27	Η	0,87817011	2,00882685	0,47684584
28	С	-0,41900125	1,71357030	0,76210194
29	С	-0,61800236	0,69009752	1,04762083
30	Η	-1,55252703	2,60363744	0,70311545
31	С	-1,34831648	3,65484068	0,89211512
32	Н	-2,85649033	2,30590509	0,46106382
33	С	-3,56242030	3,12685922	0,55157996
34	Η	-3,47017560	1,06382446	0,02192589
35	С	-4,81790714	1,06377056	-0,18704969
36	С	-5,37858613	1,97895198	-0,02599940
37	Η	-5,58649919	-0,08325130	-0,60414182
38	С	-5,05878866	-1,03450955	-0,70829400
39	Η	6,04840012	0,54363601	-1,20290342
40	С	6,58645358	0,45825696	-2,15213097
41	Н	5,71108587	1,57730889	-1,10690534
42	Н	6,75059499	0,35315904	-0,39151619
43	Н	3,98921666	-0,17943383	-2,42505005
44	С	4,56386360	-0,42230325	-3,32303941
45	Η	3,09466921	-0,80497683	-2,42220175
46	Η	3,67026476	0,86097436	-2,51329281
47	Н	3,56561467	-0,69788233	2,56098455
48	С	3,11825736	0,28924541	2,64570231
49	Η	2,78924649	-1,44662633	2,76004809
50	Η	4,31932006	-0,79831877	3,34846477
51	Η	1,32272078	3,36692810	0,01999239
52	С	0,54122481	4,11414324	0,14946253
53	Η	2,20300661	3,69040775	0,57828337
54	Η	1,59136276	3,35370720	-1,04196138
55	Н	-2,62950651	-0,16063339	-0,24429641
56	С	-3,13874965	-0,88890634	-0,86881882
57	Η	-1,71134998	0,11634470	-0,75704508
58	Η	-2,34933203	-0,65990372	0,68811702
59	Η	-7,17042089	-3,33450611	1,68642561

Sofware used for the DAM analysis

A copy of the software DAMQT1.0 for both Windows and Linux O.S. can be obtained at the Computer Physics Communications Library.

An alpha version of a new release (so far, only available for Linux O.S.) can be obtained upon request at rafael.lopez@uam.es