

Understanding the influence of the electronic structure on the crystal structure of a TTF-PTM radical dyad

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-- SUPPORTING INFORMATION --

S1 - Cartesian coordinates of the optimized polymorph structures.

Table S1. Optimized structure of 1-dim. Coordinates are given in angstrom.			
C	8.817581918	31.56039519	81.51938736
C	16.81912659	36.9261548	60.0144482
C	10.72484404	35.07883311	65.80052039
C	14.90518274	33.40976946	75.73850931
C	11.23864281	34.76538034	64.56207903
C	14.39052113	33.72532811	76.97598794
C	12.96840913	35.03106419	66.00531037
C	12.66204417	33.46558925	75.52988099
C	11.80683874	35.24732818	66.71458539
C	13.82394966	33.24463678	74.8227099
C	8.704742487	35.58606061	69.07032016
C	16.92797187	32.90453591	72.47101037
C	7.506864146	35.33677858	71.3425482
C	18.12998835	33.15851929	70.20185426
C	6.536045538	35.14934647	70.43262089
C	19.09933698	33.34349373	71.11372438
C	13.51929507	34.30728923	63.68708404
C	12.10846773	34.18791115	77.84736162
C	13.09593309	34.23543633	62.34832438
C	12.53041178	34.25784134	79.18657009
C	13.97444857	33.83921322	61.35375879
C	11.65090523	34.65097622	80.1813105
C	15.31476491	33.50274041	61.64643741
C	10.31092112	34.98788597	79.88814464
C	15.70628686	33.52556894	63.0004016
C	9.920656084	34.96687977	78.53382461
C	14.83497248	33.9276629	64.00699719
C	10.79257564	34.56695924	77.52679267
C	16.28833304	33.15061865	60.6261422
C	9.336160333	35.33875455	80.90760886
C	16.08723031	33.43761745	59.30997369
C	9.537111665	35.05592574	82.22470276
C	16.80753154	33.1230037	58.09804615

C	8.812948946	35.36902242	83.43464696
C	7.55087721	36.01888718	83.53594646
C	18.06663678	32.46790806	57.99357667
C	7.031320655	36.43036808	84.76905788
C	18.58141984	32.05481785	56.75890328
C	17.90150907	32.30051709	55.53660175
C	7.710175612	36.18992848	85.99312366
C	16.71258318	33.07148685	55.62093741
C	8.902056297	35.42281352	85.91205547
C	16.19255925	33.46767139	56.85358236
C	9.426329049	35.02762827	84.68088546
C	18.38419351	31.77426723	54.26421995
C	7.223771207	36.71930524	87.26225637
C	18.48472282	32.63875667	53.08694933
C	7.127587781	35.86141323	88.44468057
C	19.05157821	33.93983131	53.16857267
C	6.569370737	34.55605047	88.37124893
C	19.18510102	34.7641676	52.0389325
C	6.440595606	33.73808475	89.50601449
C	18.77888735	34.29571954	50.77625502
C	6.841935988	34.21756965	90.76612719
C	18.21354788	33.01087393	50.66349835
C	7.397799501	35.50705605	90.87089908
C	18.04388237	32.21191802	51.80501449
C	7.563640362	36.29967541	89.72438614
C	18.74613574	30.35417985	54.18186146
C	6.854215208	38.13793855	87.33976534
C	17.88353688	29.34977766	54.69416338
C	7.712798196	39.14608755	86.82829104
C	18.23442245	27.99110403	54.67076351
C	7.359315236	40.50402384	86.85962643
C	19.45935567	27.59224504	54.09847503
C	6.136858127	40.89796386	87.44055174
C	19.95811225	29.92144431	53.58631727
C	5.640712877	38.56502113	87.93642503
C	20.3124302	28.56271923	53.53393641
C	5.285029744	39.92283988	87.99881817
C	9.64326831	35.55554393	68.09001299
C	15.98839479	32.93221758	73.45045984
C	9.813431989	31.17939163	79.19909488
C	15.82240644	37.3080516	62.33434616
C	10.25737992	30.89421554	77.9355368
C	15.37889192	37.59268437	63.59813102
C	12.05764663	30.97147862	79.31568847
C	13.57839759	37.51858594	62.21809831
C	10.93583618	31.23009682	80.07873623
C	14.69997288	37.25915482	61.45460553
C	7.890422713	31.54031047	82.50772574
C	17.74709403	36.94593994	59.026733
C	18.94477654	37.2778926	56.77277729
C	6.693512236	31.21134378	84.76234288
C	19.91116198	37.44432222	57.69242815
C	5.726294415	31.04658568	83.84329005

C	12.43043423	30.36038836	76.89930723
C	13.20691164	38.12692934	64.63595009
C	11.79750928	30.10127923	75.6745576
C	13.84093219	38.38359593	65.86075841
C	12.53942104	29.72192839	74.57685388
C	13.10007729	38.76153124	66.95955935
C	13.93813888	29.5712628	74.63023362
C	11.70127198	38.91275552	66.90809397
C	14.56827575	29.819996	75.86581265
C	11.06996342	38.6668018	65.67233304
C	13.8306554	30.21290173	76.98284687
C	11.80675363	38.27577166	64.55384777
C	14.56714104	29.19875156	73.37636598
C	11.07543774	39.2848737	68.16405894
C	15.85582873	29.29317338	72.98730342
C	9.787842267	39.19087993	68.5567312
C	16.30664283	28.9451433	71.63746967
C	9.338198962	39.54106658	69.90647944
C	15.6274456	29.31463914	70.44673428
C	10.01630113	39.1736708	71.09842544
C	9.53267988	39.54588445	72.36147896
C	16.1087662	28.94318799	69.18272698
C	8.361040935	40.3293571	72.51107726
C	17.28123246	28.16158925	69.03049167
C	7.662534167	40.6639328	71.32504675
C	17.98061025	27.82449169	70.21537735
C	8.137265725	40.27168141	70.06885767
C	17.50699956	28.21396651	71.47297693
C	7.914617703	40.79553373	73.82771637
C	17.730911	27.70626338	67.71100809
C	7.750531707	39.865984	74.9443192
C	17.89534337	28.64757797	66.60375991
C	8.180229976	40.19403857	76.26019616
C	17.46896137	28.33340139	65.28346452
C	7.880653503	39.37612092	77.3616332
C	17.77066407	29.1631426	64.19117976
C	7.161847958	38.17903802	77.17112704
C	18.48957649	30.35792456	64.39575988
C	6.792426591	37.79064386	75.87020797
C	18.85475388	30.7328259	65.70170772
C	7.091615141	38.61961862	74.77670776
C	18.55242876	29.89272592	66.78579839
C	7.601270424	42.21970737	73.9807253
C	18.05138829	26.28513682	67.54605705
C	6.393797849	42.67079185	74.57389552
C	19.26136793	25.84521868	66.94941266
C	19.61082307	24.48456787	66.91080317
C	6.050647221	44.03335869	74.59950985
C	18.75150522	23.52191217	67.48003277
C	6.915923458	44.98680862	74.02364882
C	17.52153866	23.92704068	68.03560698
C	8.144100022	44.57056486	73.47244939
C	8.48396053	43.21058864	73.47705827

C	17.17381501	25.28521223	68.04118821
CI	6.58386441	36.26620908	82.12616106
CI	19.03548068	32.21547892	59.40130423
CI	5.452652147	37.12833897	84.80719125
CI	20.15626307	31.34816193	56.7174916
CI	15.81578065	33.41079054	54.18846496
CI	9.797553268	35.08727859	87.34632838
CI	14.71135116	34.36428492	56.85796099
CI	10.91143898	34.137638	84.67987623
CI	19.69635294	34.51423658	54.65444271
CI	5.92938803	33.96754436	86.88867033
CI	19.88439004	36.32908184	52.17926761
CI	5.753701369	32.1668281	89.37545196
CI	18.97524531	35.27391138	49.37981255
CI	6.652855813	33.24642412	92.16837384
CI	17.7100232	32.44270895	49.12328382
CI	7.895681856	36.0888173	92.40784571
CI	17.18606387	30.72941434	51.63206267
CI	8.411543852	37.78879682	89.88985127
CI	7.25370028	40.7211716	68.65381855
CI	18.39048709	27.76057409	72.88672677
CI	6.136620817	41.4667774	71.4097147
CI	19.50701847	27.02272035	70.12726886
CI	15.20422177	29.37082431	67.78012678
CI	10.43426219	39.11839728	73.76591688
CI	21.10250919	23.98929081	66.22539567
CI	4.559942475	44.54172316	75.27789239
CI	9.15692499	41.58656814	76.51935769
CI	16.49497495	26.94219182	65.00819933
CI	8.396364484	39.81242272	78.94222623
CI	17.25794218	28.74440563	62.60458338
CI	6.725059517	37.20237506	78.51471187
CI	18.932925	31.34829902	63.06407385
CI	5.925025907	36.32720594	75.62829753
CI	19.72173623	32.19323793	65.96248656
CI	6.516655117	38.13381523	73.23294889
CI	19.12397192	30.36348658	68.33516966
CI	16.29644589	29.7572062	55.21694729
CI	9.299328121	38.74509433	86.29851967
CI	17.14817757	26.80993989	55.27684021
CI	8.439879942	41.69010983	86.2528243
CI	19.89125005	25.93169475	54.07136196
CI	5.705207291	42.55835184	87.48360731
CI	21.80427264	28.07963395	52.83752709
CI	3.793456578	40.39956753	88.70061603
CI	21.08631333	31.08255779	52.99704757
CI	4.513684546	37.39825528	88.51690259
CI	5.248075103	41.5340998	75.17749623
CI	20.40338663	26.99247202	66.35872148
CI	14.17677033	30.25612153	70.51493349
CI	11.46836519	38.23407047	71.03244124
CI	19.16943035	21.86120112	67.45508606
CI	6.507340034	46.65001668	74.03471203

Cl	16.42864642	22.75539517	68.64185585
Cl	9.24441551	45.73048671	72.85757543
Cl	15.58118211	25.70592004	68.53181807
Cl	10.07397929	42.77760289	72.98829402
H	10.73600763	34.54837615	63.62833823
H	14.89330862	33.94026597	77.91014174
H	14.00718639	35.07900844	66.32202135
H	11.62350144	33.42145566	75.21182366
H	7.368837918	35.24316587	72.41864175
H	18.27129448	33.2524301	69.12630091
H	5.510035234	34.87728606	70.661374
H	20.12588441	33.61513367	70.88652429
H	12.07637311	34.50540351	62.07288681
H	13.54992803	33.98813777	79.46221083
H	13.60403596	33.7940175	60.32943665
H	12.02013999	34.69245734	81.20610128
H	16.72106258	33.21528648	63.26127385
H	8.905690671	35.27671548	78.27351187
H	15.17187553	33.91838218	65.0438261
H	10.45550394	34.57735029	76.48999322
H	17.19050529	32.65743166	60.98485231
H	8.432548166	35.8281582	80.54735897
H	15.16916267	33.98517729	59.10332257
H	10.45782427	34.51383447	82.43424034
H	9.69639851	30.79835202	77.01643601
H	15.94010038	37.68625492	64.51727241
H	13.10506098	30.91694	79.60268341
H	12.53093595	37.57547207	61.93177571
H	19.08349435	37.41282028	55.70106845
H	6.554801147	31.07658178	85.83407954
H	20.93403478	37.7344084	57.47187668
H	4.702882133	30.75857194	84.06394421
H	10.71972995	30.19950048	75.55884676
H	14.91870947	38.28481858	65.97614889
H	12.03388445	29.55943737	73.62739138
H	13.60635798	38.92253421	67.90892643
H	15.6480635	29.67765677	75.96614513
H	9.990199528	38.81034833	65.57240548
H	14.34294667	30.38806449	77.93046165
H	11.29404439	38.1041129	63.60576403
H	13.85291057	28.82784087	72.63769357
H	11.79178812	39.65607322	68.90060404
H	16.62634792	29.61397323	73.69300282
H	9.015247967	38.87014977	67.85329306
N	12.61975839	34.7247577	64.69309768
N	13.00952953	33.77129858	76.84238404
N	11.63807985	30.75191833	78.00241445
N	13.99832827	37.73666659	63.53160008
S	9.136527737	35.44442196	66.40134964
S	16.49337396	33.03878652	75.13989763
S	11.41438877	35.71483719	68.35944821
S	14.21754018	32.7727482	73.17917914
S	9.073861045	35.82586154	70.7691221

S	16.56141568	32.66966282	70.77100258
S	6.950077441	35.3935025	68.74633576
S	18.68235832	33.09436911	72.79867442
S	8.261972561	31.58905134	79.84905602
S	17.37350386	36.89598294	61.68489253
S	10.60054839	31.66406939	81.75133806
S	15.03595085	36.82457334	59.78190183
S	17.38018979	36.75237829	57.32617056
S	8.258495921	31.73487212	84.20801197
S	6.137196312	31.34697405	82.16361296
S	19.5002785	37.14109849	59.37183675

Table S2. Optimized structure of 2- <i>dim</i> . Coordinates are given in angstrom.			
C	8.464528947	30.07344917	77.99872903
C	15.77861608	35.69642407	56.17289803
C	10.54311088	34.13552578	63.27088485
C	13.71742213	31.63938219	70.89862128
C	11.08971358	33.81349691	62.0473547
C	13.17290051	31.96002835	72.1233226
C	12.77698645	33.96183409	63.55816031
C	11.48308071	31.81388546	70.61489717
C	11.59915153	34.22834604	64.22658784
C	12.65988813	31.5480795	69.94431496
C	8.440781315	34.68145412	66.48025031
C	15.81602645	31.10234155	67.68624438
C	7.187311478	34.46813383	68.72818942
C	17.07128259	31.31538094	65.43953882
C	6.227336644	34.35748827	67.79630885
C	18.03076127	31.42353996	66.37220766
C	13.37534862	33.30728904	61.22245874
C	10.88908744	32.46480824	72.95354135
C	13.04454274	33.48468114	59.86814421
C	11.22351479	32.2858624	74.30688297
C	13.90075036	33.04199758	58.87099164
C	10.3698438	32.72656187	75.30716184
C	15.12383545	32.40802668	59.17951248
C	9.145806938	33.36086508	75.00313816
C	15.44641453	32.2506943	60.54342551
C	8.819303073	33.51929246	73.64016955
C	14.59810339	32.69897708	61.55448892
C	9.664894098	33.07261183	72.62588545
C	16.01854049	31.8757025	58.15434822
C	8.254076587	33.89357735	76.03090112
C	15.96046927	32.24601893	56.85232661
C	8.317547651	33.52791902	77.33414992
C	16.63142016	31.71294107	55.67124723
C	7.648018509	34.06235687	78.5156498
C	6.398215431	34.72423668	78.56119827
C	17.88144546	31.0519242	55.62664735
C	5.886333445	35.237994	79.7667661
C	18.39443838	30.53955347	54.42097822
C	17.74089603	30.71105783	53.1820542
C	6.540773757	35.06778561	81.00540352
C	16.52317862	31.41221308	53.21146291
C	7.758113076	34.36600822	80.97536193
C	15.97568835	31.86500279	54.42019466
C	8.30415037	33.91076283	79.76676328
C	18.44232104	30.21090571	51.91816863
C	5.839503958	35.56769754	82.26960316
C	18.2729965	31.1047878	50.68391798
C	6.008087419	34.67413301	83.5042856
C	18.87944598	32.38117519	50.72963445
C	5.400100513	33.39842907	83.45925281

C	18.80900785	33.28488934	49.65419829
C	5.466622298	32.49624635	84.53625701
C	18.12220332	32.9203961	48.48634041
C	6.151886287	32.86126914	85.70488417
C	17.5367949	31.6463754	48.4015378
C	6.739853003	34.1342246	85.78854044
C	17.61635688	30.75341554	49.48819494
C	6.663409203	35.02601287	84.70066908
C	18.45435038	28.69325561	51.70550566
C	5.826327464	37.08518076	82.48305524
C	17.46624414	27.78604889	52.13632835
C	6.814016686	37.99333259	82.05344536
C	17.6423542	26.39251621	52.01880329
C	6.636852416	39.38663958	82.17197919
C	18.81901388	25.87194999	51.45026388
C	5.459375598	39.90594739	82.74003402
C	19.6008769	28.14300657	51.09060094
C	4.679388823	37.63414571	83.09838451
C	19.79695527	26.75713094	50.96055587
C	4.482333225	39.01975388	83.22966063
C	9.396366512	34.61947644	65.51957479
C	14.86115187	31.16148726	68.64768049
C	9.5725375	29.43835668	75.77864537
C	14.67464313	36.33241662	58.39369732
C	10.09174479	29.0802694	74.55728853
C	14.15833018	36.69252861	59.61550435
C	11.81667375	29.32945481	76.01035375
C	12.43025043	36.44425915	58.16569669
C	10.64914114	29.5937124	76.70113934
C	13.59628478	36.17770076	57.47308264
C	7.506005571	30.20739922	78.94828378
C	16.73656304	35.56405687	55.22252345
C	17.99552334	35.81384627	52.99498423
C	6.249407159	29.96072446	81.17768701
C	18.93814572	36.00083924	53.93294052
C	5.30589915	29.77116629	80.24113678
C	12.34387924	28.67155864	73.64316143
C	11.90940831	37.10333829	60.53477975
C	11.8899825	28.81290742	72.32366811
C	12.36799447	36.96126712	61.85268093
C	12.667687	28.36192355	71.27271406
C	11.59449317	37.41235766	62.90661718
C	13.94237007	27.79926047	71.48483656
C	10.31916272	37.97521328	62.69923825
C	14.424502	27.74039494	72.8061893
C	9.832154454	38.03453628	61.37967444
C	13.63363529	28.16063566	73.87821659
C	10.61901549	37.61462995	60.30451823
C	14.62138332	27.30266931	70.29455721
C	9.644487807	38.47110781	63.89235895
C	15.93364506	27.30972603	69.98548291
C	8.333463048	38.46167729	64.2061985
C	16.47142686	26.91281345	68.67743079

C	7.798253581	38.85999105	65.51486265
C	15.84511304	27.19213254	67.43720321
C	8.426851559	38.58350896	66.75456889
C	7.843351429	38.94444122	67.98288239
C	16.42879001	26.8305158	66.20925669
C	6.626236791	39.64463819	68.04389926
C	17.64585972	26.13021354	66.14875842
C	5.995758243	39.92132063	66.81379809
C	18.27552639	25.85322693	67.37918941
C	6.55247438	39.52116503	65.58999209
C	17.71711161	26.2513029	68.6028998
C	5.913756499	40.07068793	69.32627248
C	18.35999928	25.70654602	64.86657276
C	6.046297454	39.11747335	70.51934649
C	18.22830387	26.66217139	63.67538679
C	6.662191806	39.41491944	71.75114855
C	17.61495255	26.36721542	62.44172668
C	6.631708627	38.50812505	72.82922298
C	17.64654686	27.27687214	61.36598483
C	5.978965085	37.27137395	72.69262391
C	18.29766383	28.51401239	61.50704621
C	5.381012026	36.93732559	71.46799381
C	18.892997	28.8454093	62.73365503
C	5.415463372	37.85784204	70.40587503
C	18.85753377	27.92214568	63.79324982
C	5.911540563	41.57894384	69.60081609
C	18.36392	24.19880459	64.58970037
C	4.757817549	42.12009959	70.20958172
C	19.5191473	23.65958131	63.98216232
C	19.72230412	22.2754971	63.84368864
C	4.556778059	43.50452021	70.34775219
C	18.74629736	21.38287955	64.32442061
C	5.53343102	44.39558688	69.86552067
C	17.5602506	21.89268612	64.88289644
C	6.717548194	43.88388101	69.30470078
C	6.906163572	42.49200475	69.19576216
C	17.36971338	23.2842665	64.9923361
CI	5.426500909	34.86502358	77.14054007
CI	18.85068295	30.90941025	57.04878044
CI	4.36759327	36.06051895	79.72379543
CI	19.91246096	29.71603218	54.46460814
CI	15.60259211	31.64942297	51.77382361
CI	8.678858227	34.12927205	82.41295759
CI	14.39077852	32.54024763	54.39066702
CI	9.887103273	33.23067765	79.79741559
CI	19.75611088	32.86798575	52.12833482
CI	4.525600654	32.91099675	82.05939146
CI	19.58071956	34.82006946	49.73989594
CI	4.691771811	30.96248394	84.45180467
CI	18.00832237	34.01154261	47.16576108
CI	6.26067307	31.77228421	87.02770916
CI	16.69789635	31.20125071	46.96980109
CI	7.57745306	34.57962855	87.22098443

CI	16.79547056	29.25370225	49.32591626
CI	7.485218428	36.52528934	84.86310192
CI	5.711554951	39.87129351	64.12333664
CI	18.55646962	25.89943229	70.06982511
CI	4.479527856	40.74860829	66.78804514
CI	19.79335411	25.02865086	67.40558581
CI	15.55490232	27.18390398	64.76597379
CI	8.718054163	38.59195557	69.42593825
CI	21.16302872	21.67092414	63.13417925
CI	3.117927652	44.11154793	71.05923462
CI	7.551355837	40.86744284	71.96934308
CI	16.7278005	24.91414406	62.21855484
CI	7.409887452	38.89009214	74.31395412
CI	16.87195518	26.89776871	59.87862777
CI	5.896594101	36.18479444	74.01964461
CI	18.38160721	29.60472713	60.18346429
CI	4.579932419	35.42562901	71.29582262
CI	19.69281704	30.35698065	62.91137762
CI	4.619825619	37.42234114	68.94399485
CI	19.65067237	28.35460029	65.25733323
CI	15.94010607	28.33168991	52.71290931
CI	8.34073951	37.4487796	81.47748782
CI	16.40251274	25.32248601	52.52937964
CI	7.876440793	40.4580144	81.66363651
CI	19.04728844	24.17296446	51.33325998
CI	5.228925146	41.60469734	82.8561307
CI	21.23152004	26.14165111	50.24805012
CI	3.047782612	39.6336056	83.94371429
CI	20.82000829	29.19708465	50.47131751
CI	3.460799459	36.57888236	83.71665962
CI	3.532787017	41.05578618	70.79962776
CI	20.74383899	24.72595289	63.39507514
CI	14.31384253	27.97479486	67.38280898
CI	9.961520279	37.8073545	66.80762479
CI	18.97331253	19.68776509	64.18789841
CI	5.309661558	46.09106424	70.00335048
CI	16.32639026	20.81212122	65.38558777
CI	7.951563653	44.9625814	68.79847057
CI	15.82237089	23.81673063	65.51973196
CI	8.452301374	41.95757567	68.66658497
H	10.62158928	33.64415989	61.086119
H	13.64292189	32.1279136	73.08394236
H	13.80687921	33.9317352	63.91004058
H	10.45266782	31.84437447	70.26435589
H	7.015829442	34.34856195	69.79734983
H	17.24438794	31.43551586	64.37076299
H	5.188208661	34.12195746	67.99983693
H	19.07050389	31.65702976	66.16960792
H	12.11801726	33.98683193	59.58901044
H	12.15103415	31.78386911	74.58284098
H	13.60002919	33.18041042	57.83135122
H	10.67345533	32.58609227	76.34569583
H	16.37606906	31.74154449	60.81086124

H	7.888847334	34.02874375	73.3761864
H	14.86414071	32.5412941	62.60141175
H	9.395814095	33.23124906	71.57987866
H	16.72277932	31.11654555	58.49560242
H	7.546804536	34.65002362	75.69006847
H	15.23544315	33.02315722	56.60696169
H	9.045589015	32.75359003	77.57967532
H	19.5019004	30.39492036	52.16933322
H	4.780063065	35.38333727	82.01815369
H	9.594614358	28.86332947	73.62151547
H	14.65767238	36.91003842	60.54995066
H	12.85651848	29.34012552	76.33317025
H	11.38992902	36.43517648	57.844411
H	18.16032252	35.93879897	51.92530614
H	6.086221932	29.83719775	82.24776919
H	19.95906241	36.3193103	53.73979612
H	4.28528441	29.45248603	80.43582913
H	10.93494979	29.29339179	72.11375769
H	13.32308338	36.47948461	62.05912054
H	12.30166248	28.47291526	70.25179609
H	11.96402291	37.30054376	63.92615846
H	15.39762241	27.2844056	73.00608007
H	8.858044682	38.49024517	61.1837993
H	13.99408456	28.04124915	74.90237313
H	10.25480949	37.7340766	59.28161494
H	13.92497773	26.9389417	69.53852697
H	10.34321232	38.83627468	64.64554401
H	16.66847726	27.64176219	70.72401575
H	7.597113715	38.1271098	63.4703522
H	4.855666197	39.91013814	69.05130096
H	19.41763045	25.86754782	65.14309923
N	12.46031408	33.70086166	62.22732051
N	11.80193286	32.07323689	71.94573938
N	11.4676002	29.01273544	74.6988057
N	12.78225623	36.76178775	59.47645431
S	8.947737976	34.56471464	63.81174691
S	15.31184361	31.21027758	70.35502897
S	11.161212	34.68921325	65.8639077
S	13.09634028	31.08991935	68.3055516
S	8.795736709	34.86813023	68.18998767
S	15.46128082	30.91956361	65.97604655
S	6.687962066	34.61566693	66.12580661
S	17.56822597	31.1658257	68.04208026
S	7.987651153	29.90358891	76.30857529
S	16.2576743	35.86300058	57.86304736
S	10.23773409	30.15543477	78.31373197
S	14.00519934	35.61451681	55.86000952
S	16.41792264	35.28518148	53.52069666
S	7.825796778	30.49038506	80.64907094
S	5.758903396	30.069832	78.56998992
S	18.48310113	35.69955211	55.60302897

Table S3. Optimized structure of 1-hb . Coordinates are given in angstrom.			
C	26.16207512	16.5496106	74.20753352
C	26.83534611	20.58285355	70.84945418
C	24.56462422	16.89280205	72.22748713
C	28.4381312	20.92078251	72.82645285
C	23.77697257	17.0368339	71.10340654
C	29.22863873	21.06419095	73.94851308
C	22.71973152	15.59947535	72.51660804
C	30.27933565	19.62275113	72.53460195
C	23.90602461	15.98238353	73.1101966
C	29.09234126	20.00779027	71.94315107
C	27.30627377	16.48310527	74.94930173
C	25.68958154	20.52121115	70.10938796
C	29.2547185	15.70748819	76.46240809
C	23.73808085	19.75567632	68.59430614
C	29.78815888	16.65468919	75.66940829
C	23.20704082	20.70018431	69.39203681
C	21.62380144	16.06643593	70.33197243
C	31.38135909	20.09218044	74.7169554
C	21.90557328	16.20144998	68.95934078
C	31.10093749	20.22943257	76.08966363
C	20.90664709	16.00337488	68.01692285
C	32.10112486	20.03532764	77.03148755
C	19.59310852	15.6601374	68.4086468
C	33.41496251	19.69367145	76.63940198
C	19.33288205	15.5469127	69.79030059
C	33.67378343	19.57743497	75.25765141
C	20.32444957	15.74054582	70.74282065
C	32.6807904	19.7672467	74.30555798
C	18.50845442	15.39898091	67.47859476
C	34.50049555	19.43691386	77.57003671
C	18.59839913	15.35623415	66.12550499
C	34.40931136	19.39472649	78.92314992
C	17.51696901	15.03631589	65.20387127
C	35.48976265	19.0778831	79.84715375
C	16.17789581	15.48621138	65.33770965
C	36.82798876	19.53110824	79.71609353
C	15.19215032	15.15384443	64.40122777
C	37.81286434	19.20072756	80.65425305
C	15.43528836	14.23169786	63.34094916
C	37.56985035	18.27778254	81.71383696
C	16.78811961	13.82324724	63.17568746
C	36.21759135	17.86697102	81.87705628
C	17.79390796	14.26557052	64.04332079
C	35.212322	18.30704147	81.0075565
C	14.34714008	13.69928674	62.53511734
C	38.65811856	17.74578084	82.51999245
C	14.46191826	13.49691404	61.0903941
C	38.54475566	17.54306154	83.96482878
C	14.02172656	12.29758517	60.47233688
C	38.98714916	16.34403232	84.58209464

C	14.0906777	12.11409232	59.08125844
C	38.92457262	16.16181012	85.97363029
C	14.64376727	13.12242639	58.26811092
C	38.37511734	17.17089562	86.78829392
C	15.08951999	14.32362717	58.85116001
C	37.92606809	18.3712413	86.20600056
C	14.98214568	14.50817479	60.23752069
C	38.02665838	18.55434874	84.81890458
C	13.09416975	13.34026314	63.21438641
C	39.91097012	17.38679792	81.84023729
C	13.09819516	12.54691618	64.39087918
C	39.90635681	16.59262539	80.66434953
C	11.91786524	12.27286365	65.09732883
C	41.08636787	16.31751418	79.95779548
C	10.681303	12.71361032	64.58962664
C	42.32325717	16.7580385	80.46488674
C	10.63917176	13.43453739	63.38313483
C	42.36599935	17.47964446	81.67093622
C	11.83460841	13.7660031	62.72542928
C	41.17081997	17.81237054	82.32857347
C	17.9965852	20.56220569	70.84697985
C	35.00251207	16.5331912	74.20499066
C	32.67459982	16.05619269	73.22583243
C	20.32555487	20.091403	71.82746534
C	31.44151166	15.72307737	72.69933385
C	21.55838101	19.76021342	72.35597944
C	32.57034242	16.9298688	71.13281921
C	20.4313861	20.97879905	73.91473135
C	33.37733311	16.82376072	72.24654319
C	19.6239738	20.86628525	72.80185522
C	16.84545735	20.47689457	70.11750761
C	36.15257111	16.45556568	74.93682394
C	14.36570251	20.5404556	69.3760399
C	38.63222107	16.52857339	75.67681172
C	38.02234981	15.72181178	76.56370026
C	14.9773284	19.7292826	68.49446733
C	30.32816454	16.098017	70.50177217
C	22.67179748	20.145518	74.55183155
C	28.99869022	16.09382882	70.93582823
C	24.00157766	20.12948016	74.11871513
C	27.97658457	16.00268517	69.99784903
C	25.02255805	20.03917718	75.05801592
C	28.24114422	15.92067458	68.6147973
C	24.75715421	19.96869358	76.44161268
C	29.59493397	15.87534534	68.20663995
C	23.40287605	19.93627625	76.84931402
C	30.6201276	15.96005086	69.13329478
C	22.37880741	20.02066124	75.92133755
C	27.12405054	15.9473466	67.68878301
C	25.87458267	19.99206825	77.36746447
C	27.23888579	16.05968374	66.33923784
C	25.76184007	20.10466658	78.71726245
C	26.18995089	16.2709754	65.361454

C	26.8127237	20.3124351	79.69399016
C	26.49626945	17.008817	64.18109372
C	26.50954216	21.04915291	80.87596487
C	25.51243495	17.42671204	63.27974413
C	27.49551166	21.46454651	81.77623764
C	24.15897997	17.01269483	63.42032926
C	28.84818209	21.04893995	81.63305243
C	23.90026893	16.09391336	64.48120381
C	29.1038799	20.13130753	80.57046786
C	24.85498567	15.79261936	65.45769682
C	28.14697638	19.83231338	79.59527573
C	23.08366996	17.54648234	62.60619718
C	29.92560065	21.58050172	82.44604569
C	21.82762968	17.90510299	63.276951
C	31.18062941	21.93946518	81.7737518
C	21.82335224	18.68337546	64.46388338
C	31.18311501	22.71947985	80.58794318
C	20.63403073	18.97742877	65.14770118
C	32.37149779	23.01577196	79.90354161
C	19.39948778	18.57509328	64.60482761
C	33.60697207	22.61532118	80.44569014
C	19.36854787	17.84556016	63.40331502
C	33.63973432	21.88423292	81.64621491
C	20.57021879	17.49600858	62.76766354
C	32.43898165	21.53090757	82.28142699
C	23.2116855	17.75962078	61.16501794
C	29.80131964	21.79164846	83.8879064
C	22.77742191	18.96369958	60.55213323
C	30.2396627	22.99386532	84.50180324
C	22.84579614	19.15327336	59.16207283
C	30.17740935	23.18026027	85.89259547
C	23.3955557	18.1466235	58.34463044
C	29.62904315	22.17279934	86.70996772
C	23.84308272	16.94394931	58.92308597
C	29.17781377	20.97192706	86.13057264
C	23.73668696	16.75349759	60.30867991
C	29.27836667	20.78443798	84.7441453
CI	15.75512252	16.58599139	66.60810821
CI	37.24941553	20.6330253	78.44732976
CI	13.681368	15.99133699	64.4601942
CI	39.32219845	20.04099776	80.59831877
CI	17.19891603	12.65884725	61.97919621
CI	35.80774123	16.70172469	83.07298107
CI	19.4219086	13.78269236	63.73217037
CI	33.58478291	17.82124197	81.31638206
CI	13.48908235	10.96522134	61.43115453
CI	39.51463688	15.01054867	83.62201801
CI	13.55474915	10.64684361	58.36992071
CI	39.46449493	14.69546307	86.68399332
CI	14.77142851	12.90096495	56.57732116
CI	38.25463967	16.95099108	88.47981586
CI	15.70105284	15.57825644	57.84693113
CI	37.31945257	19.62691699	87.21188843

CI	15.36588594	16.05844503	60.87001442
CI	37.63763204	20.10333301	84.18647712
CI	28.12907997	17.48913402	63.87780343
CI	24.87801436	21.53134214	81.18306374
CI	25.94220293	18.58013822	62.07714227
CI	27.06962308	22.61745861	82.98072355
CI	22.39966975	15.23644157	64.50213082
CI	30.60392037	19.27288833	80.54537022
CI	24.39713101	14.71748527	66.73505851
CI	28.60150631	18.7580911	78.31590311
CI	23.28014876	19.4280787	65.01278219
CI	29.72537334	23.46425434	80.04165971
CI	20.65485421	19.89372444	66.60543068
CI	32.34790914	23.93283128	78.44631198
CI	17.94363155	19.02089562	65.38241604
CI	35.06176392	23.06592839	79.66913836
CI	17.86404956	17.36682984	62.73168031
CI	35.14553438	21.4092365	82.31756334
CI	20.48788749	16.48883194	61.37713203
CI	32.52391823	20.52134778	83.67011585
CI	14.55252457	11.76663007	64.8895138
CI	38.45168603	15.81180554	80.16737745
CI	11.94716052	11.33429121	66.54154605
CI	41.05624244	15.37713999	78.51476379
CI	9.237153208	12.34389339	65.42733426
CI	43.76694841	16.38688832	79.62700968
CI	9.128833614	13.9232572	62.73302298
CI	43.87682483	17.96714987	82.32084361
CI	11.74198882	14.77785899	61.3383543
CI	41.26427399	18.82507947	83.71496151
CI	22.25496675	20.29465823	61.51930505
CI	30.76052765	24.32625286	83.53574363
CI	22.31395133	20.6254401	58.45763117
CI	30.71561812	24.64962197	86.59836516
CI	23.51959386	18.37315398	56.65401392
CI	29.51102528	22.39591458	88.40150272
CI	24.45545643	15.69355126	57.91323738
CI	28.56853934	19.71989771	87.1402187
CI	24.13229233	15.20385151	60.93574368
CI	28.87882693	19.23643936	84.11525266
H	29.80780668	15.15984407	77.22476772
H	23.18365646	19.21201304	67.83008174
H	23.90570691	17.64342111	70.21522589
H	29.1038708	21.67274354	74.83589704
H	30.632063	15.10969736	73.08101632
H	22.36703499	19.14346081	71.977971
H	21.95699796	14.89166866	72.82319151
H	31.04011791	18.91321063	72.22706019
H	32.7122212	17.44715201	70.19110782
H	20.29010652	21.50212531	74.85328884
H	13.3010841	20.77960268	69.36732294
H	39.69654582	16.76910522	75.68337654
H	30.83354848	16.96679126	75.68310076

H	22.16215952	21.01403774	69.38084046
H	38.52266677	15.23049785	77.39738985
H	14.47855711	19.23240986	67.66315995
H	22.92364947	16.41443119	68.6326524
H	30.08288865	20.44149788	76.41704705
H	28.7646083	16.21396577	71.99447064
H	24.23717443	20.23967884	73.05938786
H	21.16167344	16.08747722	66.95905199
H	31.84696238	20.12176153	78.08937649
H	26.94043534	16.03774846	70.34176959
H	26.05904482	20.06485105	74.71427472
H	18.32182122	15.3047934	70.12379003
H	34.68491595	19.33609074	74.92374047
H	29.85619989	15.76829494	67.15268193
H	23.14011343	19.83942412	77.90388629
H	20.08285641	15.6691279	71.80347837
H	32.92133226	19.69346885	73.24479529
H	31.65850818	15.89719687	68.80974768
H	21.34002929	19.96688344	76.24496358
H	17.5507179	15.17040677	67.95269606
H	35.45928673	19.21097869	77.09673893
H	26.13926308	15.95760507	68.158756
H	26.85900845	19.99796737	76.89672087
H	19.57790622	15.48578609	65.65965445
H	33.42877546	19.52155761	79.38756872
H	28.24581846	16.1267339	65.92573827
H	24.75566322	20.17448975	79.13214338
N	22.65004737	16.24529977	71.28704284
N	30.3533382	20.26986059	73.76331347
N	31.39065457	16.25666359	71.41893406
N	21.61028638	20.30202479	73.63300938
S	26.06039598	17.59481808	72.77903159
S	26.94407075	21.62784797	72.27732213
S	24.70280591	15.64196255	74.62366753
S	28.29030989	19.66882217	70.43160951
S	27.53662249	15.40743787	76.33340062
S	25.45567366	19.45240071	68.72053553
S	28.70500907	17.5036859	74.59545908
S	24.29206581	21.54164915	70.46985136
S	33.49408812	15.77453915	74.73844196
S	19.50470088	19.80049983	70.31716998
S	34.93982627	17.44913227	72.69098928
S	18.06194014	21.4902209	72.35311076
S	15.36379828	21.32553163	70.57364453
S	37.63186152	17.30513178	74.47532838
S	36.29238014	15.52257946	76.42892248
S	16.70728214	19.53344305	68.63183035

Table S4. Optimized structure of 2-hb . Coordinates are given in angstrom.			
C	26.51211982	16.66219985	74.41300219
C	27.11306766	20.75613257	70.9596684
C	24.91491836	17.02649244	72.4386153
C	28.7124451	21.10640943	72.93481489
C	24.13030393	17.18491224	71.31444228
C	29.49945797	21.25977469	74.05785189
C	23.10760491	15.67010059	72.67028094
C	30.51734774	19.7481706	72.69486131
C	24.27849682	16.0677512	73.28466589
C	29.34558295	20.14937824	72.08441163
C	27.65862765	16.58560182	75.14732683
C	25.96728566	20.68913377	70.22333975
C	29.63004236	15.76500794	76.60586534
C	23.99133238	19.88162073	68.76423013
C	30.14578691	16.74953229	75.84753135
C	23.47998103	20.86469923	69.52745613
C	22.00804559	16.18654547	70.49592693
C	31.61842894	20.25309634	74.87103499
C	22.28739287	16.39787315	69.13240736
C	31.33428059	20.45042223	76.235586
C	21.29396594	16.22399487	68.178313
C	32.32520981	20.2700995	77.1907431
C	19.9913001	15.82603448	68.54821011
C	33.62997348	19.87957796	76.82053663
C	19.73335033	15.63053172	69.91968053
C	33.89254837	19.69716045	75.44809992
C	20.7180531	15.80330266	70.88461722
C	32.91014253	19.87657532	74.48192623
C	18.90876831	15.59677409	67.6024289
C	34.70986259	19.64638032	77.76804549
C	18.98137315	15.64361629	66.25246536
C	34.63356436	19.69124925	79.11790527
C	17.86711968	15.37030323	65.33952862
C	35.74508716	19.41687517	80.03325758
C	16.5652536	15.90175021	65.48816148
C	37.04798162	19.94588055	79.88592068
C	15.56300422	15.65113013	64.53617656
C	38.04895982	19.69308295	80.83835912
C	15.74223348	14.73296675	63.47673629
C	37.8665621	18.77653137	81.89854984
C	17.03228059	14.19082288	63.33184032
C	36.57475821	18.23844021	82.0436374
C	18.07788659	14.56714852	64.19528918
C	35.53093569	18.61600062	81.17852934
C	14.53566146	14.44759403	62.58071556
C	39.07264404	18.48898749	82.79456415
C	14.78119206	13.98930221	61.14102617
C	38.82577856	18.03488822	84.23515748
C	14.45059643	12.72131849	60.62790611
C	39.15671556	16.76878528	84.75236243

C	14.52634725	12.43889298	59.24871068
C	39.0791735	16.4902124	86.13224009
C	15.01083065	13.41350472	58.35853032
C	38.59260482	17.46698123	87.0188695
C	15.3858271	14.67441402	58.84766981
C	38.21738162	18.72623669	86.52559494
C	15.2525658	14.95159904	60.21903309
C	38.35224804	18.9995732	85.15363955
C	13.34424086	13.79104706	63.290253
C	40.26122718	17.82814688	82.08385786
C	13.42060643	12.96252357	64.42839533
C	40.17997674	16.9982498	80.94701579
C	12.26197769	12.55772917	65.11944571
C	41.33542714	16.59186635	80.25164764
C	10.99096141	12.90199967	64.62790389
C	42.60872691	16.93628996	80.7371719
C	10.88665717	13.64759028	63.44316327
C	42.71807805	17.6815918	81.92171716
C	12.05447177	14.10900615	62.81249119
C	41.55312133	18.14424075	82.55694268
C	18.32529657	20.83840949	70.97934594
C	35.2779608	16.71307013	74.38473731
C	32.94760674	16.2456464	73.40804447
C	20.65125566	20.3404948	71.95359033
C	31.71262959	15.91503181	72.88600279
C	21.88427405	19.99799817	72.47384699
C	32.85749029	17.07760739	71.29822225
C	20.7501121	21.16468729	74.06618865
C	33.66070571	16.98635418	72.41686046
C	19.94559016	21.08421546	72.9479129
C	17.18186963	20.77243773	70.24161998
C	36.41894949	16.62663432	75.12405267
C	14.70458958	20.81871952	69.49622213
C	38.89140579	16.64810428	75.88907898
C	38.25373284	15.87024478	76.78155039
C	15.32849802	20.03954444	68.59526636
C	30.60334319	16.25375682	70.68422288
C	22.99879647	20.32910445	74.67672097
C	29.27598664	16.31804045	71.1173342
C	24.32650174	20.40047849	74.24595731
C	28.24892952	16.21683494	70.18412817
C	25.35242464	20.30149825	75.18080155
C	28.51211639	16.05755747	68.80982884
C	25.08790442	20.13702068	76.55426291
C	29.86058095	15.94018258	68.40519568
C	23.73931556	20.01297068	76.95643781
C	30.89080505	16.03394086	69.32600089
C	22.71021743	20.10453945	76.03402003
C	27.39760143	16.08994947	67.87609462
C	26.20122001	20.17035012	77.48955716
C	27.50706845	16.11578366	66.52713899
C	26.0908594	20.19018412	78.83847965
C	26.42995284	16.32229065	65.56388269

C	27.16755661	20.39539178	79.80276788
C	26.68304096	17.11297963	64.4149107
C	26.91398123	21.18473434	80.95240207
C	25.66913232	17.47890393	63.51224192
C	27.92723714	21.54875247	81.85651024
C	24.3766571	16.93611902	63.62022974
C	29.21916144	21.00465728	81.74939218
C	24.16600515	16.01701893	64.6727997
C	29.4301813	20.08635909	80.6961113
C	25.12870863	15.77576221	65.66617498
C	28.46848199	19.84795376	79.70101149
C	23.19081211	17.23750618	62.70636272
C	30.40439567	21.30442684	82.66441139
C	21.99928143	17.90458449	63.40578287
C	31.59741656	21.96890576	81.96519544
C	22.07090579	18.72377216	64.55098873
C	31.52794906	22.78715295	80.81913966
C	20.90830289	19.15455213	65.21987617
C	32.69190685	23.21225198	80.14898262
C	19.64060498	18.84256007	64.6992296
C	33.95867364	22.89587338	80.66926597
C	19.54220722	18.08545414	63.52137901
C	34.05513145	22.14011497	81.84810871
C	20.71224699	17.60726952	62.90784225
C	32.88356589	21.66748759	82.4629237
C	23.4605925	17.70495679	61.27476407
C	30.13425887	21.77292821	84.09549561
C	23.1391107	18.97675877	60.76598604
C	30.45500097	23.04528468	84.6033632
C	23.22010692	19.26357186	59.38827603
C	30.37169985	23.33359489	85.98062165
C	23.70534021	18.29042979	58.49691883
C	29.88603127	22.36106236	86.87240774
C	24.08061978	17.02871625	58.98371669
C	29.51217437	21.09852052	86.3865526
C	23.94103781	16.74676883	60.35339758
C	29.65330989	20.81539295	85.01726875
CI	16.19880852	16.95685652	66.80760085
CI	37.41824154	21.00139578	78.56775654
CI	14.06624113	16.51400656	64.67452489
CI	39.54810572	20.55131416	80.69938059
CI	17.35971132	12.9713856	62.16309517
CI	36.24330718	17.02239018	83.2148315
CI	19.66721318	13.97234693	63.88052304
CI	33.93932391	18.02639218	81.49245921
CI	14.03553516	11.41465956	61.67561732
CI	39.57534019	15.45975109	83.70900497
CI	14.06713686	10.8975899	58.65391827
CI	39.53919562	14.95107436	86.73203766
CI	15.15007262	13.07738934	56.68482135
CI	38.45137021	17.13556785	88.69328137
CI	15.94752299	15.88301662	57.76092909
CI	37.65405171	19.93766749	87.6083444

CI	15.63205655	16.54325446	60.74874668
CI	37.97167722	20.58922755	84.61858694
CI	28.27982472	17.71457006	64.14020393
CI	25.31778693	21.78800515	81.22583292
CI	26.0319116	18.69144648	62.34493181
CI	27.56429938	22.76059717	83.02442593
CI	22.66812533	15.15164032	64.76314433
CI	30.9269999	19.21838396	80.60734594
CI	24.70461725	14.73343909	66.97591421
CI	28.89294171	18.80817503	78.38940431
CI	23.57669738	19.35181235	65.11151599
CI	30.02397959	23.41962732	80.25841081
CI	21.01643468	20.10599389	66.64820659
CI	32.58707768	24.16234183	78.71950307
CI	18.23285839	19.41632303	65.48064969
CI	35.36796586	23.46345465	79.88606296
CI	18.0032331	17.74682593	62.8436885
CI	35.59333945	21.79595187	82.52499082
CI	20.53960203	16.64757008	61.48442891
CI	33.05316029	20.70793273	83.88676585
CI	14.92602039	12.30494504	64.95029612
CI	38.6722747	16.34032436	80.43288409
CI	12.37267647	11.60282367	66.54631668
CI	41.21778299	15.63357964	78.82755499
CI	9.587040476	12.40146669	65.46587641
CI	44.00914356	16.43591816	79.89274955
CI	9.342602488	13.98963605	62.77784548
CI	44.26493073	18.02115566	82.58170597
CI	11.87504629	15.08117164	61.39789688
CI	41.73854684	19.11526895	83.97158638
CI	22.73046005	20.28207191	61.81869064
CI	30.86502198	24.3495242	83.54993016
CI	22.76471099	20.80717903	58.7969162
CI	30.82433493	24.87843772	86.57085864
CI	23.84511194	18.63027774	56.82434032
CI	29.7438853	22.7027195	88.54439348
CI	24.64849849	15.82395712	57.89576906
CI	28.94332148	19.89460395	87.4749009
CI	24.32625716	15.15684202	60.88314523
CI	29.26872692	19.22488654	84.48843196
H	30.19816163	15.18408958	77.33165525
H	23.41980119	19.30467972	68.03794475
H	24.24678389	17.82544131	70.44868641
H	29.38652132	21.8979975	74.92566573
H	30.89773498	15.31480658	73.27623438
H	22.69511811	19.39400202	72.08077467
H	22.36208535	14.93378014	72.95114243
H	31.26194446	19.01237865	72.4101838
H	33.00494001	17.57751838	70.34760888
H	20.6083815	21.66379451	75.01800618
H	13.63524063	21.03435887	69.49667544
H	39.96197049	16.85796741	75.89964879
H	31.19042834	17.0655959	75.85659265

H	22.43589714	21.18267409	69.52276088
H	38.73278544	15.37486169	77.62509412
H	14.83871692	19.5488433	67.75521186
H	23.2998434	16.65568649	68.82135493
H	30.31996324	20.70180767	76.54583804
H	29.04857572	16.49915361	72.16894402
H	24.55483685	20.5860814	73.19526103
H	21.54345397	16.37266904	67.12634993
H	32.07193871	20.4074903	78.24330219
H	27.21501951	16.30778782	70.52459336
H	26.38631937	20.39857864	74.84223051
H	18.72959901	15.34247684	70.23778542
H	34.89796883	19.41456051	75.13032684
H	30.11186499	15.77483679	67.35671739
H	23.48706244	19.84494818	78.00431133
H	20.47491858	15.66976172	71.93872979
H	33.15593094	19.75353797	73.42713787
H	31.92708864	15.92163127	69.00951146
H	21.67372008	19.98839915	76.34857706
H	17.95615786	15.32466161	68.06561949
H	35.66342025	19.37481349	77.30660154
H	26.41368829	16.17819311	68.34174839
H	27.18535776	20.26389141	77.02533376
H	19.94527995	15.824759	65.77008534
H	33.66854614	19.87267917	79.59787658
H	28.5059187	16.10343065	66.08765558
H	25.09190822	20.17271377	79.27769627
N	23.02563252	16.35490258	71.46275959
N	30.60239408	20.42876511	73.90426138
N	31.66957947	16.42290182	71.59555421
N	21.93232035	20.50139631	73.76592625
S	26.37821003	17.76744556	73.03173178
S	27.25046023	21.85348846	72.34684375
S	25.06974226	15.71441561	74.8008415
S	28.55110561	19.80362933	70.56844515
S	27.90917217	15.46387874	76.49341108
S	25.71189745	19.57555389	68.87145575
S	29.04125827	17.64191924	74.83089894
S	24.59004105	21.7506905	70.54413288
S	33.75603432	15.98617677	74.93129566
S	19.83902678	20.0971389	70.42874464
S	35.22565495	17.61527372	72.86003518
S	18.3888736	21.73389223	72.50713881
S	15.69100427	21.60253162	70.70606741
S	37.92203622	17.44099447	74.67172207
S	36.51797483	15.72008876	76.63771864
S	17.06512156	19.88162444	68.72051845
H	14.14412802	15.46839389	62.41303048
H	22.78913647	16.2230129	62.52502841
H	39.46748168	19.50888319	82.96025042
H	30.80418731	20.28933691	82.8464535