

## Electronic Supporting Information (ESI)

### A computational study of a light-driven artificial device: a third generation rotational photo-molecular motor in dilute solutions

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Supplementary Information sections are organized as follows: first, we have introduced the optimized molecular geometries as obtained by the application of several Density Functionals (B3LYP, Cam-B3LYP, PBE, PBE0) in conjunction with the Conductor-like and Polarizable Continuum model (C-PCM), then we report the applied all-atoms topology files used for simulating the artificial rotor in different rotamers via a classical molecular dynamics (MD) framework in acetonitrile dilute solution.

#### Quantum mechanics optimized structures and Molecular Dynamics files (gro e itp):

In this section we share the optimized molecular structures obtained considering the investigated molecular motor in three different conformations: stable and meta-stable product. Moreover, we also report the files used for simulating the investigated motor in acetonitrile dilute solution at room temperature (gro and itp files for the selected OPLS-AAA mechanical force field):

#### Cam-B3LYP(D3)/ 6-311+g\*\*/most-stable rotamer/C-PCM(ACN)

6	1.202747	-0.275047	0.340607
6	-0.000003	0.673925	0.041353
6	-1.202773	-0.275009	0.340646
6	-0.697924	-1.307828	1.244611
6	0.697893	-1.307855	1.244587
6	1.401444	-2.041448	2.200937
6	0.699336	-2.793706	3.124201
6	-0.699373	-2.793680	3.124223
6	-1.401478	-2.041393	2.200979
6	-0.000019	1.044104	-1.446427
1	2.481161	-1.995243	2.241860
1	1.235589	-3.356816	3.878158

1	-1.235624	-3.356767	3.878197
1	-2.481192	-1.995142	2.241930
6	0.000032	1.878981	1.003433
1	-0.000041	0.126701	-2.034882
1	0.880323	1.616642	-1.725156
1	-0.880350	1.616669	-1.725133
6	-0.000010	3.190708	0.535134
6	0.000021	4.270646	1.410522
6	0.000095	4.059430	2.780504
6	0.000139	2.756503	3.263446
6	0.000109	1.681887	2.386328
1	-0.000072	3.391603	-0.528296
1	-0.000015	5.278305	1.012533
1	0.000119	4.898465	3.465594
1	0.000198	2.572213	4.331194
1	0.000145	0.679833	2.793825
6	-2.457465	-0.243767	-0.176467
6	-3.328898	-1.438130	-0.393902
6	-4.532607	-1.023200	-0.990004
6	-4.502314	0.428581	-1.135344
6	-3.255916	0.900077	-0.681414
6	-3.043934	2.273605	-0.626649
6	-4.026216	3.143055	-1.086669
6	-5.235965	2.660464	-1.578816
6	-5.484946	1.293959	-1.591707
1	-5.990860	3.352403	-1.932348
1	-3.847309	4.211073	-1.050708
1	-6.437651	0.911707	-1.939136
1	-2.137957	2.682022	-0.212710
6	-3.073552	-2.803877	-0.291324
6	-4.038423	-3.716935	-0.698030
6	-5.252730	-3.289476	-1.231728
6	-5.498609	-1.933575	-1.395201
1	-2.134624	-3.172663	0.093919
1	-3.837071	-4.777334	-0.603624
1	-5.993835	-4.016918	-1.540260
1	-6.420768	-1.591863	-1.850520
6	2.457433	-0.243814	-0.176522
6	3.328847	-1.438183	-0.393997
6	3.255908	0.900037	-0.681422
6	4.532593	-1.023248	-0.990017
6	4.502326	0.428539	-1.135301
6	5.498593	-1.933626	-1.395216
6	5.252668	-3.289528	-1.231834
6	4.038321	-3.716989	-0.698229
6	3.073454	-2.803930	-0.291520
1	5.993769	-4.016973	-1.540371
1	3.836936	-4.777389	-0.603902
1	2.134491	-3.172708	0.093647
1	6.420782	-1.591913	-1.850472
6	3.043932	2.273564	-0.626658
6	4.026246	3.143015	-1.086613
6	5.236020	2.660423	-1.578696
6	5.484989	1.293916	-1.591596
1	6.437708	0.911661	-1.938984
1	5.990940	3.352362	-1.932177
1	3.847341	4.211032	-1.050651
1	2.137934	2.681988	-0.212773

**Cam-B3LYP(D3)/ 6-311+g\*\*/Phe-orth rotamer/C-PCM (ACN)**

6	1.190217	0.198743	0.297655
6	0.000019	-0.784461	0.094057
6	-1.190196	0.198737	0.297620

6	0.697848	1.184870	1.266371
6	-0.698829	2.585791	3.206889
6	-0.697857	1.184875	1.266339
6	-1.402724	1.875481	2.250008
1	-2.483123	1.834850	2.282860
6	2.413188	0.205496	-0.284960
6	3.200813	-0.906963	-0.889717
6	3.287349	1.408336	-0.428986
6	2.972924	-2.277841	-0.991668
6	4.456457	-0.407868	-1.288376
6	3.033158	2.763673	-0.235463
6	4.495391	1.029206	-1.035668
6	3.955890	-3.106393	-1.520753
1	2.049262	-2.724984	-0.664164
6	5.439337	-1.233816	-1.811535
6	4.005993	3.698701	-0.567148
1	2.089311	3.106824	0.161303
6	5.470351	1.960468	-1.364665
6	5.180732	-2.592354	-1.935438
1	3.761880	-4.168932	-1.604439
1	6.398061	-0.826376	-2.110129
6	5.225961	3.303156	-1.112226
1	3.806491	4.751204	-0.404934
1	6.397398	1.647458	-1.830509
1	5.935462	-3.253892	-2.343229
1	5.973190	4.046954	-1.361269
1	-1.234944	3.118427	3.982853
6	-2.413164	0.205488	-0.285002
6	-3.287311	1.408338	-0.429004
6	-3.200825	-0.906964	-0.889733
6	-3.033096	2.763666	-0.235447
6	-4.495356	1.029239	-1.035695
6	-2.972988	-2.277853	-0.991653
6	-4.456454	-0.407835	-1.288403
6	-4.005910	3.698719	-0.567125
1	-2.089245	3.106788	0.161335
6	-5.470294	1.960526	-1.364686
6	-3.955979	-3.106380	-1.520731
1	-2.049348	-2.725027	-0.664131
6	-5.439358	-1.233759	-1.811555
6	-5.225880	3.303205	-1.112224
1	-3.806391	4.751215	-0.404890
1	-6.397348	1.647541	-1.830535
6	-5.180799	-2.592306	-1.935437
1	-3.762005	-4.168928	-1.604395
1	-6.398069	-0.826292	-2.110155
1	-5.973093	4.047021	-1.361259
1	-5.935549	-3.253826	-2.343221
6	0.698741	2.585776	3.206927
1	1.234825	3.118402	3.982921
6	1.402675	1.875457	2.250082
1	2.483072	1.834810	2.282990
6	0.000066	-1.424439	-1.315779
1	0.000073	-2.511913	-1.277756
1	-0.869285	-1.111601	-1.884740
1	0.869456	-1.111592	-1.884678
6	0.000002	-1.803846	1.259764
6	-1.193514	-2.262529	1.816939
6	1.193500	-2.262501	1.817000
6	-1.196261	-3.184956	2.855245
1	-2.140339	-1.884082	1.459730
6	1.196215	-3.184928	2.855307
1	2.140334	-1.884031	1.459839
6	-0.000030	-3.659760	3.374465

1	-2.140927	-3.522200	3.265215
1	2.140869	-3.522149	3.265325
1	-0.000043	-4.376851	4.186510

**Cam-B3LYP(D3)/ 6-311+g\*\*/most-stable rotamer/C-PCM(CHX)**

6	1.202920	-0.272310	0.347206
6	0.000015	0.675914	0.044427
6	-1.203094	-0.272049	0.347292
6	-0.697951	-1.302153	1.254476
6	0.697631	-1.302316	1.254416
6	1.401132	-2.033757	2.212421
6	0.699019	-2.783777	3.137326
6	-0.699523	-2.783622	3.137380
6	-1.401540	-2.033443	2.212530
6	0.000032	1.038774	-1.445280
1	2.480991	-1.986976	2.250877
1	1.235534	-3.345174	3.892580
1	-1.236104	-3.344900	3.892674
1	-2.481386	-1.986421	2.251069
6	0.000262	1.886396	0.998607
1	-0.000074	0.118666	-2.029310
1	0.881713	1.608373	-1.726616
1	-0.881535	1.608559	-1.726596
6	0.001452	3.195163	0.522464
6	0.001722	4.280256	1.390832
6	0.000815	4.077479	2.761687
6	-0.000342	2.778003	3.252206
6	-0.000599	1.698237	2.382239
1	0.002215	3.387161	-0.542642
1	0.002655	5.285825	0.987201
1	0.001024	4.920629	3.441689
1	-0.001042	2.600407	4.321084
1	-0.001494	0.698292	2.794823
6	-2.456818	-0.244283	-0.171009
6	-3.325541	-1.440496	-0.389451
6	-4.526052	-1.028646	-0.993233
6	-4.497479	0.422841	-1.140903
6	-3.255295	0.897110	-0.680223
6	-3.047169	2.270384	-0.620181
6	-4.028261	3.137835	-1.085324
6	-5.232743	2.653063	-1.586489
6	-5.478541	1.286432	-1.602019
1	-5.987143	3.343714	-1.943665
1	-3.853559	4.206395	-1.044208
1	-6.428696	0.902361	-1.954374
1	-2.146548	2.678681	-0.194544
6	-3.068075	-2.805090	-0.283326
6	-4.028643	-3.720639	-0.693333
6	-5.239957	-3.296460	-1.234700
6	-5.486952	-1.941737	-1.402259
1	-2.129578	-3.170344	0.106294
1	-3.825636	-4.780543	-0.596755
1	-5.977724	-4.025843	-1.546683
1	-6.406573	-1.602563	-1.864560
6	2.456647	-0.244643	-0.171078
6	3.325322	-1.440881	-0.389565
6	3.255170	0.896744	-0.680215
6	4.525880	-1.029035	-0.993260
6	4.497364	0.422464	-1.140850
6	5.486765	-1.942139	-1.402297
6	5.239706	-3.296863	-1.234839
6	4.028346	-3.721031	-0.693564
6	3.067794	-2.805471	-0.283545

1	5.977459	-4.026254	-1.546834
1	3.825293	-4.780933	-0.597069
1	2.129262	-3.170713	0.106004
1	6.406422	-1.602972	-1.864531
6	3.047050	2.270019	-0.620141
6	4.028185	3.137468	-1.085196
6	5.232691	2.652691	-1.586303
6	5.478467	1.286055	-1.601876
1	6.428634	0.901982	-1.954197
1	5.987122	3.343343	-1.943411
1	3.853496	4.206030	-1.044061
1	2.146396	2.678313	-0.194557

**Cam-B3LYP(D3)/ 6-311+g\*\*/Phe-orth rotamer/C-PCM (CHX)**

6	1.190785	0.200767	0.295670
6	0.000101	-0.781650	0.092618
6	-1.190198	0.201412	0.295119
6	0.698096	1.189223	1.261895
6	-0.698322	2.594642	3.198597
6	-0.697325	1.189702	1.261468
6	-1.402062	1.882652	2.243412
1	-2.482488	1.841556	2.274916
6	2.414217	0.205778	-0.285494
6	3.201380	-0.907962	-0.888176
6	3.290193	1.407162	-0.428954
6	2.971401	-2.278089	-0.990425
6	4.458691	-0.411123	-1.283188
6	3.036551	2.762687	-0.239138
6	4.499229	1.025748	-1.031180
6	3.954058	-3.108428	-1.516262
1	2.046014	-2.722448	-0.664173
6	5.440833	-1.239201	-1.802947
6	4.011198	3.695946	-0.568576
1	2.090704	3.106454	0.152240
6	5.475539	1.955542	-1.358059
6	5.180473	-2.596842	-1.927374
1	3.758457	-4.170677	-1.600183
1	6.401070	-0.833410	-2.098882
6	5.232162	3.298390	-1.108468
1	3.811791	4.749026	-0.409998
1	6.403345	1.640896	-1.821272
1	5.935152	-3.259818	-2.332977
1	5.980792	4.041068	-1.356669
1	-1.234637	3.128242	3.973900
6	-2.413690	0.206791	-0.285932
6	-3.288739	1.408744	-0.430280
6	-3.202046	-0.906948	-0.887112
6	-3.033933	2.764227	-0.241721
6	-4.498111	1.027824	-1.032131
6	-2.973641	-2.277493	-0.987330
6	-4.458895	-0.409339	-1.282650
6	-4.007786	3.698021	-0.571988
1	-2.087761	3.107544	0.149268
6	-5.473637	1.958151	-1.359833
6	-3.957168	-3.107482	-1.512091
1	-2.048838	-2.722452	-0.660269
6	-5.441901	-1.237052	-1.801359
6	-5.229102	3.301019	-1.111489
1	-3.807465	4.751076	-0.414397
1	-6.401743	1.643868	-1.822690
6	-5.182980	-2.595123	-1.924024
1	-3.762742	-4.170066	-1.594482
1	-6.401740	-0.830645	-2.097738

1	-5.977106	4.044109	-1.360344
1	-5.938368	-3.257835	-2.328739
6	0.698970	2.594192	3.198983
1	1.235205	3.127459	3.974571
6	1.402768	1.881740	2.244190
1	2.483151	1.839968	2.276255
6	0.000664	-1.420852	-1.317728
1	0.000238	-2.508461	-1.279340
1	-0.868402	-1.108029	-1.887189
1	0.870726	-1.108735	-1.886076
6	-0.000567	-1.802055	1.257440
6	-1.194236	-2.262745	1.812007
6	1.192362	-2.260414	1.815515
6	-1.197326	-3.187982	2.847224
1	-2.140575	-1.882975	1.455106
6	1.194213	-3.185640	2.850747
1	2.139000	-1.878744	1.461459
6	-0.001852	-3.663233	3.366369
1	-2.142336	-3.526494	3.255373
1	2.138678	-3.522285	3.261692
1	-0.002340	-4.382437	4.176566

**B3LYP(D3)/ 6-311+g\*\*/most-stable rotamer/C-PCM(ACN)**

6	1.208127	-0.274380	0.362539
6	-0.000010	0.668633	0.033045
6	-1.208065	-0.274484	0.362515
6	-0.703938	-1.289645	1.277686
6	0.704066	-1.289583	1.277700
6	1.408848	-2.026842	2.240679
6	0.703062	-2.776820	3.170183
6	-0.702845	-2.776873	3.170175
6	-1.408676	-2.026951	2.240660
6	-0.000021	1.002402	-1.469779
1	2.489322	-1.984102	2.278779
1	1.238863	-3.337793	3.926987
1	-1.238612	-3.337886	3.926973
1	-2.489154	-1.984295	2.278744
6	-0.000104	1.904539	0.966530
1	0.000017	0.070077	-2.036038
1	0.882218	1.569041	-1.760024
1	-0.882305	1.568970	-1.760026
6	-0.000510	3.209535	0.461529
6	-0.000609	4.316229	1.311865
6	-0.000309	4.140748	2.692733
6	0.000083	2.845663	3.211885
6	0.000178	1.743927	2.359909
1	-0.000763	3.383560	-0.606828
1	-0.000925	5.313558	0.886893
1	-0.000387	4.998134	3.355825
1	0.000314	2.689376	4.284831
1	0.000481	0.752523	2.793486
6	-2.474944	-0.247544	-0.159741
6	-3.332322	-1.448672	-0.386098
6	-4.545839	-1.039818	-0.990236
6	-4.525745	0.411746	-1.129446
6	-3.275606	0.892026	-0.662767
6	-3.070052	2.272738	-0.604525
6	-4.057674	3.142283	-1.069521
6	-5.268354	2.653283	-1.570930
6	-5.512937	1.279873	-1.589015
1	-6.024807	3.343225	-1.927220

1	-3.883228	4.211669	-1.030964
1	-6.463274	0.895507	-1.942515
1	-2.166948	2.683785	-0.185556
6	-3.063814	-2.818224	-0.286013
6	-4.021343	-3.743395	-0.701658
6	-5.242587	-3.324205	-1.242776
6	-5.503018	-1.964709	-1.404493
1	-2.122839	-3.178153	0.104882
1	-3.810381	-4.802773	-0.608655
1	-5.975538	-4.058595	-1.556801
1	-6.426902	-1.632087	-1.864496
6	2.475001	-0.247398	-0.159731
6	3.332401	-1.448516	-0.386047
6	3.275648	0.892171	-0.662795
6	4.545905	-1.039669	-0.990212
6	4.525790	0.411888	-1.129472
6	5.503093	-1.964563	-1.404443
6	5.242682	-3.324057	-1.242670
6	4.021450	-3.743242	-0.701522
6	3.063913	-2.818068	-0.285903
1	5.975640	-4.058449	-1.556673
1	3.810504	-4.802619	-0.608476
1	2.122945	-3.177993	0.105015
1	6.426969	-1.631946	-1.864466
6	3.070092	2.272884	-0.604595
6	4.057702	3.142421	-1.069629
6	5.268378	2.653416	-1.571039
6	5.512970	1.280008	-1.589081
1	6.463306	0.895636	-1.942577
1	6.024823	3.343352	-1.927359
1	3.883248	4.211807	-1.031104
1	2.166995	2.683942	-0.185626

**B3LYP(D3)/ 6-311+g\*\*/Phe-orth rotamer/C-PCM (ACN)**

6	1.195378	0.194451	0.307742
6	-0.000038	-0.789008	0.082693
6	-1.195437	0.194446	0.307816
6	0.703453	1.163206	1.288368
6	-0.702154	2.552518	3.250600
6	-0.703471	1.163200	1.288415
6	-1.409540	1.850285	2.282994
1	-2.490563	1.811880	2.313924
6	2.429322	0.207367	-0.279921
6	3.219789	-0.898343	-0.889580
6	3.292673	1.417643	-0.421353
6	2.995634	-2.275237	-1.006336
6	4.482098	-0.388387	-1.289499
6	3.026977	2.776384	-0.224026
6	4.512383	1.047064	-1.032162
6	3.985265	-3.100158	-1.542951
1	2.071476	-2.728056	-0.686522
6	5.470987	-1.213476	-1.818756
6	3.995825	3.724424	-0.553828
1	2.079591	3.110232	0.174263
6	5.482521	1.993420	-1.358634
6	5.215098	-2.577530	-1.952930
1	3.793238	-4.162902	-1.637140
1	6.429517	-0.801860	-2.114425
6	5.225039	3.338774	-1.101317
1	3.787276	4.775456	-0.388752
1	6.413099	1.690595	-1.825566

1	5.972580	-3.234326	-2.365142
1	5.966813	4.090044	-1.347352
1	-1.238007	3.077799	4.032661
6	-2.429379	0.207351	-0.279844
6	-3.292810	1.417574	-0.421219
6	-3.219732	-0.898369	-0.889612
6	-3.027215	2.776324	-0.223813
6	-4.512496	1.046934	-1.032043
6	-2.995419	-2.275222	-1.006514
6	-4.482090	-0.388498	-1.289482
6	-3.996139	3.724307	-0.553555
1	-2.079855	3.110218	0.174497
6	-5.482707	1.993235	-1.358455
6	-3.984970	-3.100196	-1.543194
1	-2.071199	-2.727963	-0.686760
6	-5.470898	-1.213642	-1.818802
6	-5.225327	3.338594	-1.101060
1	-3.787671	4.775346	-0.388417
1	-6.413262	1.690368	-1.825405
6	-5.214867	-2.577658	-1.953102
1	-3.792830	-4.162911	-1.637493
1	-6.429471	-0.802098	-2.114433
1	-5.967159	4.089822	-1.347047
1	-5.972283	-3.234496	-2.365369
6	0.702239	2.552520	3.250559
1	1.238135	3.077803	4.032590
6	1.409572	1.850291	2.282911
1	2.490597	1.811891	2.313781
6	-0.000150	-1.411377	-1.342634
1	-0.000088	-2.500122	-1.318405
1	-0.870851	-1.090119	-1.906937
1	0.870376	-1.090013	-1.907142
6	0.000027	-1.830877	1.239687
6	-1.198181	-2.297310	1.795650
6	1.198298	-2.296837	1.795911
6	-1.200823	-3.235781	2.826983
1	-2.145610	-1.912742	1.446033
6	1.201086	-3.235305	2.827246
1	2.145649	-1.911882	1.446509
6	0.000171	-3.719182	3.342621
1	-2.146303	-3.576964	3.233787
1	2.146613	-3.576109	3.234260
1	0.000227	-4.446404	4.146552

**B3LYP(D3)/ 6-311+g\*\*/most-stable rotamer/C-PCM(CHX )**

6	1.208398	-0.274231	0.367454
6	0.000004	0.668009	0.035213
6	-1.208511	-0.274071	0.367510
6	-0.704018	-1.287654	1.284565
6	0.703822	-1.287756	1.284523
6	1.408449	-2.023471	2.248837
6	0.702750	-2.771939	3.179441
6	-0.703046	-2.771838	3.179483
6	-1.408693	-2.023270	2.248919
6	0.000010	0.996030	-1.468927
1	2.489074	-1.980126	2.284894
1	1.238822	-3.331810	3.937141
1	-1.239153	-3.331634	3.937214
1	-2.489309	-1.979772	2.285040
6	0.000163	1.908244	0.961730
1	-0.000055	0.061819	-2.031852
1	0.883423	1.560227	-1.761089



1	-0.883335	1.560338	-1.761075
6	0.000950	3.210453	0.450054
6	0.001125	4.321424	1.294183
6	0.000521	4.153276	2.675574
6	-0.000246	2.861392	3.201131
6	-0.000413	1.755418	2.355468
1	0.001456	3.376698	-0.619593
1	0.001741	5.316894	0.864412
1	0.000656	5.014114	3.334223
1	-0.000712	2.710922	4.274932
1	-0.001005	0.765877	2.793291
6	-2.474866	-0.248613	-0.154726
6	-3.331267	-1.450411	-0.382616
6	-4.541146	-1.042349	-0.993629
6	-4.521053	0.409127	-1.133540
6	-3.274517	0.890129	-0.660119
6	-3.071206	2.270271	-0.594996
6	-4.056845	3.139542	-1.063469
6	-5.262941	2.650336	-1.573919
6	-5.505857	1.277111	-1.596362
1	-6.018349	3.340291	-1.932582
1	-3.885385	4.209213	-1.018541
1	-6.454224	0.892540	-1.954952
1	-2.172652	2.679836	-0.164865
6	-3.062987	-2.819318	-0.280124
6	-4.017736	-3.745079	-0.699609
6	-5.235354	-3.326810	-1.247715
6	-5.494773	-1.967914	-1.412212
1	-2.123118	-3.177925	0.114659
1	-3.806729	-4.804376	-0.605305
1	-5.966225	-4.061671	-1.565604
1	-6.415775	-1.635905	-1.878476
6	2.474755	-0.248831	-0.154771
6	3.331136	-1.450641	-0.382663
6	3.274426	0.889904	-0.660131
6	4.541038	-1.042586	-0.993635
6	4.520970	0.408895	-1.133521
6	5.494661	-1.968159	-1.412208
6	5.235215	-3.327054	-1.247742
6	4.017575	-3.745313	-0.699675
6	3.062829	-2.819545	-0.280198
1	5.966083	-4.061921	-1.565622
1	3.806550	-4.804609	-0.605394
1	2.122945	-3.178142	0.114557
1	6.415682	-1.636157	-1.878441
6	3.071110	2.270047	-0.595009
6	4.056770	3.139315	-1.063443
6	5.262882	2.650106	-1.573854
6	5.505794	1.276879	-1.596303
1	6.454169	0.892307	-1.954869
1	6.018305	3.340060	-1.932487
1	3.885312	4.208987	-1.018519
1	2.172533	2.679611	-0.164916

**B3LYP(D3)/ 6-311+g\*\*/Phe-orth rotamer/C-PCM (CHX)**

6	1.208398	-0.274231	0.367454
6	0.000004	0.668009	0.035213
6	-1.208511	-0.274071	0.367510
6	-0.704018	-1.287654	1.284565
6	0.703822	-1.287756	1.284523
6	1.408449	-2.023471	2.248837

6	0.702750	-2.771939	3.179441
6	-0.703046	-2.771838	3.179483
6	-1.408693	-2.023270	2.248919
6	0.000010	0.996030	-1.468927
1	2.489074	-1.980126	2.284894
1	1.238822	-3.331810	3.937141
1	-1.239153	-3.331634	3.937214
1	-2.489309	-1.979772	2.285040
6	0.000163	1.908244	0.961730
1	-0.000055	0.061819	-2.031852
1	0.883423	1.560227	-1.761089
1	-0.883335	1.560338	-1.761075
6	0.000950	3.210453	0.450054
6	0.001125	4.321424	1.294183
6	0.000521	4.153276	2.675574
6	-0.000246	2.861392	3.201131
6	-0.000413	1.755418	2.355468
1	0.001456	3.376698	-0.619593
1	0.001741	5.316894	0.864412
1	0.000656	5.014114	3.334223
1	-0.000712	2.710922	4.274932
1	-0.001005	0.765877	2.793291
6	-2.474866	-0.248613	-0.154726
6	-3.331267	-1.450411	-0.382616
6	-4.541146	-1.042349	-0.993629
6	-4.521053	0.409127	-1.133540
6	-3.274517	0.890129	-0.660119
6	-3.071206	2.270271	-0.594996
6	-4.056845	3.139542	-1.063469
6	-5.262941	2.650336	-1.573919
6	-5.505857	1.277111	-1.596362
1	-6.018349	3.340291	-1.932582
1	-3.885385	4.209213	-1.018541
1	-6.454224	0.892540	-1.954952
1	-2.172652	2.679836	-0.164865
6	-3.062987	-2.819318	-0.280124
6	-4.017736	-3.745079	-0.699609
6	-5.235354	-3.326810	-1.247715
6	-5.494773	-1.967914	-1.412212
1	-2.123118	-3.177925	0.114659
1	-3.806729	-4.804376	-0.605305
1	-5.966225	-4.061671	-1.565604
1	-6.415775	-1.635905	-1.878476
6	2.474755	-0.248831	-0.154771
6	3.331136	-1.450641	-0.382663
6	3.274426	0.889904	-0.660131
6	4.541038	-1.042586	-0.993635
6	4.520970	0.408895	-1.133521
6	5.494661	-1.968159	-1.412208
6	5.235215	-3.327054	-1.247742
6	4.017575	-3.745313	-0.699675
6	3.062829	-2.819545	-0.280198
1	5.966083	-4.061921	-1.565622
1	3.806550	-4.804609	-0.605394
1	2.122945	-3.178142	0.114557
1	6.415682	-1.636157	-1.878441
6	3.071110	2.270047	-0.595009
6	4.056770	3.139315	-1.063443
6	5.262882	2.650106	-1.573854
6	5.505794	1.276879	-1.596303
1	6.454169	0.892307	-1.954869
1	6.018305	3.340060	-1.932487
1	3.885312	4.208987	-1.018519
1	2.172533	2.679611	-0.164916

**PBE0(D3)/ 6-311+g\*\*/most-stable rotamer/C-PCM(ACN )**

6	1.199740	-0.278990	0.348897
6	0.000001	0.659182	0.034476
6	-1.199734	-0.278999	0.348891
6	-0.701826	-1.304113	1.250553
6	0.701834	-1.304107	1.250560
6	1.406684	-2.048196	2.202839
6	0.701112	-2.805273	3.121925
6	-0.701113	-2.805279	3.121917
6	-1.406681	-2.048207	2.202825
6	0.000008	1.018574	-1.452611
1	2.488721	-2.003362	2.242978
1	1.236827	-3.373542	3.874877
1	-1.236831	-3.373554	3.874864
1	-2.488719	-2.003382	2.242950
6	-0.000006	1.870994	0.985018
1	0.000011	0.095896	-2.036336
1	0.883931	1.590820	-1.733228
1	-0.883911	1.590820	-1.733238
6	-0.000062	3.180050	0.500615
6	-0.000067	4.270509	1.366294
6	-0.000017	4.072367	2.740709
6	0.000037	2.772497	3.238258
6	0.000042	1.686690	2.371593
1	-0.000103	3.367321	-0.567983
1	-0.000110	5.275522	0.957072
1	-0.000021	4.919724	3.418256
1	0.000076	2.599254	4.309645
1	0.000086	0.685634	2.788100
6	-2.465065	-0.242388	-0.168474
6	-3.325395	-1.433332	-0.391994
6	-4.534983	-1.018475	-0.988763
6	-4.507093	0.429452	-1.124800
6	-3.256067	0.898923	-0.664847
6	-3.040466	2.274726	-0.603520
6	-4.021520	3.149031	-1.062006
6	-5.234134	2.670179	-1.558567
6	-5.488371	1.302408	-1.577975
1	-5.987731	3.366793	-1.911071
1	-3.839959	4.218234	-1.021609
1	-6.443977	0.925143	-1.928579
1	-2.130771	2.678821	-0.184461
6	-3.062646	-2.800944	-0.296965
6	-4.024649	-3.717228	-0.709150
6	-5.243390	-3.291804	-1.241606
6	-5.497222	-1.934525	-1.399730
1	-2.119484	-3.166859	0.088559
1	-3.818162	-4.778885	-0.620202
1	-5.982154	-4.022716	-1.553696
1	-6.422403	-1.596009	-1.855644
6	2.465070	-0.242376	-0.168470
6	3.325406	-1.433317	-0.391988
6	3.256064	0.898935	-0.664859
6	4.534996	-1.018457	-0.988749
6	4.507097	0.429468	-1.124797
6	5.497242	-1.934505	-1.399705
6	5.243414	-3.291783	-1.241582
6	4.024669	-3.717212	-0.709138
6	3.062659	-2.800930	-0.296962
1	5.982183	-4.022694	-1.553665
1	3.818184	-4.778869	-0.620192

1	2.119494	-3.166848	0.088552
1	6.422425	-1.595986	-1.855613
6	3.040448	2.274737	-0.603561
6	4.021497	3.149043	-1.062054
6	5.234121	2.670195	-1.558596
6	5.488371	1.302426	-1.577978
1	6.443982	0.925164	-1.928572
1	5.987715	3.366810	-1.911105
1	3.839925	4.218245	-1.021679
1	2.130745	2.678832	-0.184520

**PBE0(D3)/ 6-311+g\*\*/ Phe-orth rotamer/C-PCM(ACN )**

6	1.187443	0.205062	0.298944
6	0.000015	-0.771135	0.088170
6	-1.187009	0.205374	0.298973
6	0.701744	1.189044	1.260517
6	-0.699736	2.607726	3.192079
6	-0.701078	1.189007	1.260782
6	-1.407011	1.890931	2.240028
1	-2.489606	1.850973	2.273242
6	2.420292	0.201958	-0.284763
6	3.196922	-0.912460	-0.878828
6	3.288509	1.398434	-0.434861
6	2.961247	-2.285782	-0.973464
6	4.459210	-0.419745	-1.282853
6	3.032635	2.757223	-0.249406
6	4.500943	1.014220	-1.041232
6	3.941326	-3.123127	-1.498331
1	2.031796	-2.726154	-0.643490
6	5.438963	-1.257264	-1.800800
6	4.006724	3.691597	-0.586601
1	2.085687	3.101900	0.146112
6	5.476567	1.947166	-1.375363
6	5.171402	-2.616967	-1.916140
1	3.741207	-4.186682	-1.576907
1	6.402141	-0.857663	-2.102174
6	5.229726	3.292699	-1.129190
1	3.806288	4.746674	-0.430788
1	6.405776	1.633119	-1.840401
1	5.923549	-3.286354	-2.320533
1	5.977850	4.037027	-1.381571
1	-1.235388	3.146398	3.966612
6	-2.419750	0.202455	-0.284890
6	-3.288428	1.398727	-0.434475
6	-3.195680	-0.911832	-0.880003
6	-3.033133	2.757581	-0.248619
6	-4.500776	1.014235	-1.040859
6	-2.958913	-2.284830	-0.976376
6	-4.458302	-0.419549	-1.283451
6	-4.007699	3.691638	-0.585305
1	-2.086287	3.102587	0.146831
6	-5.476896	1.946861	-1.374450
6	-3.938470	-3.122320	-1.501989
1	-2.028950	-2.724840	-0.647314
6	-5.437552	-1.257222	-1.802093
6	-5.230641	3.292404	-1.127784
1	-3.807683	4.746747	-0.429168
1	-6.406007	1.632569	-1.839518
6	-5.169043	-2.616619	-1.918905
1	-3.737516	-4.185619	-1.581889
1	-6.401020	-0.857957	-2.102985
1	-5.979143	4.036492	-1.379752

1	-5.920770	-3.286112	-2.323900
6	0.700975	2.607929	3.191712
1	1.236872	3.146753	3.965970
6	1.407970	1.891258	2.239360
1	2.490582	1.851474	2.272158
6	-0.000654	-1.410783	-1.318024
1	-0.001987	-2.500468	-1.280322
1	-0.873540	-1.095355	-1.886084
1	0.872925	-1.097492	-1.886155
6	-0.000774	-1.783506	1.258171
6	-1.197506	-2.236925	1.818902
6	1.194836	-2.236153	1.821921
6	-1.200833	-3.152676	2.865721
1	-2.145030	-1.856867	1.456531
6	1.196074	-3.151904	2.868761
1	2.143042	-1.855610	1.461885
6	-0.002887	-3.624080	3.390220
1	-2.147372	-3.486468	3.278848
1	2.141775	-3.485112	3.284274
1	-0.003698	-4.335857	4.209242

**PBEPBE (D3)/ 6-311+g\*\*/ Phe-orth rotamer/C-PCM(ACN )**

6	1.195702	0.194471	0.320848
6	0.000151	-0.784001	0.086631
6	-1.195789	0.194189	0.320529
6	0.708728	1.162696	1.301004
6	-0.706393	2.570618	3.261915
6	-0.709334	1.162716	1.300593
6	-1.418666	1.861706	2.294252
1	-2.508847	1.823578	2.326475
6	2.440012	0.202976	-0.275251
6	3.222637	-0.903686	-0.886349
6	3.296008	1.414795	-0.423697
6	2.994706	-2.287558	-0.998194
6	4.489870	-0.392273	-1.300426
6	3.025715	2.778741	-0.223236
6	4.519575	1.045075	-1.047785
6	3.983869	-3.118194	-1.541645
1	2.062427	-2.741027	-0.668804
6	5.477746	-1.225799	-1.835476
6	3.992567	3.733743	-0.563190
1	2.072065	3.111262	0.187310
6	5.486896	2.000613	-1.383613
6	5.216829	-2.595705	-1.963624
1	3.788281	-4.189136	-1.632838
1	6.443249	-0.815087	-2.141634
6	5.224281	3.350530	-1.122470
1	3.779956	4.792305	-0.395882
1	6.422649	1.700749	-1.862291
1	5.976144	-3.260048	-2.382622
1	5.967041	4.110559	-1.375888
1	-1.245697	3.103749	4.048046
6	-2.440067	0.202458	-0.275631
6	-3.296219	1.414186	-0.423458
6	-3.222802	-0.904203	-0.886595
6	-3.026050	2.778012	-0.222099
6	-4.519703	1.044650	-1.047776
6	-2.995090	-2.288124	-0.998305
6	-4.490012	-0.392659	-1.300669
6	-3.992897	3.733124	-0.561752
1	-2.072512	3.110318	0.188917

6	-5.486990	2.000308	-1.383363
6	-3.984390	-3.118659	-1.541675
1	-2.062865	-2.741730	-0.668937
6	-5.478002	-1.226087	-1.835650
6	-5.224453	3.350118	-1.121551
1	-3.780411	4.791609	-0.393804
1	-6.422673	1.700615	-1.862284
6	-5.217272	-2.596040	-1.963712
1	-3.788939	-4.189635	-1.632772
1	-6.443486	-0.815265	-2.141718
1	-5.967202	4.110237	-1.374726
1	-5.976689	-3.260315	-2.382633
6	0.704507	2.570418	3.262485
1	1.243318	3.103425	4.049039
6	1.417396	1.861421	2.295330
1	2.507540	1.823132	2.328413
6	0.000610	-1.407299	-1.337101
1	0.001387	-2.504672	-1.313890
1	-0.879652	-1.084104	-1.903829
1	0.880516	-1.082877	-1.903723
6	0.000551	-1.824967	1.247616
6	-1.203806	-2.291944	1.806019
6	1.205348	-2.290375	1.806319
6	-1.205408	-3.232599	2.843341
1	-2.158098	-1.902180	1.449823
6	1.207899	-3.230991	2.843677
1	2.159234	-1.899382	1.450347
6	0.001500	-3.716358	3.361529
1	-2.157920	-3.575814	3.254659
1	2.160755	-3.572890	3.255295
1	0.001880	-4.447624	4.173182

**PBEPBE(D3)/ 6-311+g\*\*/most-stable rotamer/C-PCM(ACN )**

6	1.209068	-0.276563	0.373475
6	-0.000369	0.656657	0.028660
6	-1.208679	-0.277019	0.373303
6	-0.709378	-1.289501	1.289637
6	0.710216	-1.289132	1.289824
6	1.417741	-2.038983	2.251449
6	0.706481	-2.795725	3.179873
6	-0.706140	-2.795843	3.179867
6	-1.417222	-2.039233	2.251220
6	-0.000270	0.983841	-1.475701
1	2.507591	-1.996674	2.288406
1	1.245663	-3.365143	3.940448
1	-1.245147	-3.365271	3.940538
1	-2.507051	-1.996476	2.287708
6	-0.000724	1.901903	0.953762
1	-0.001102	0.042982	-2.043546
1	0.892068	1.551922	-1.769244
1	-0.891712	1.553520	-1.768831
6	0.000708	3.207469	0.431370
6	0.000382	4.327529	1.273794
6	-0.001449	4.164683	2.662103
6	-0.003019	2.870043	3.196707
6	-0.002675	1.754336	2.353741
1	0.001715	3.365163	-0.649293
1	0.001567	5.328579	0.835602
1	-0.001779	5.035503	3.321568
1	-0.004572	2.724071	4.279666
1	-0.003924	0.757682	2.798807
6	-2.488936	-0.245283	-0.150847
6	-3.337071	-1.448277	-0.384279

6	-4.556598	-1.040053	-0.996771
6	-4.540071	0.413281	-1.128160
6	-3.285380	0.894865	-0.649674
6	-3.078224	2.281422	-0.580350
6	-4.067484	3.156800	-1.046598
6	-5.280246	2.668746	-1.559608
6	-5.527734	1.290214	-1.587414
1	-6.040471	3.366771	-1.918147
1	-3.893251	4.234460	-0.997981
1	-6.485482	0.907596	-1.949593
1	-2.168932	2.691301	-0.145962
6	-3.060405	-2.822469	-0.287024
6	-4.014512	-3.754719	-0.712563
6	-5.239882	-3.338259	-1.260729
6	-5.508532	-1.974365	-1.421086
1	-2.110583	-3.180046	0.111639
1	-3.796408	-4.821572	-0.622472
1	-5.972626	-4.081506	-1.583658
1	-6.438900	-1.644449	-1.890529
6	2.489108	-0.244622	-0.151052
6	3.337550	-1.447629	-0.383915
6	3.285541	0.895457	-0.650114
6	4.557008	-1.039488	-0.996679
6	4.540320	0.413822	-1.128565
6	5.509123	-1.973983	-1.420296
6	5.240848	-3.337793	-1.258543
6	4.015578	-3.754117	-0.710035
6	3.061153	-2.821700	-0.285520
1	5.973902	-4.081160	-1.580506
1	3.797915	-4.820961	-0.618861
1	2.111050	-3.178932	0.112777
1	6.439256	-1.644411	-1.890466
6	3.078387	2.282012	-0.580950
6	4.067685	3.157383	-1.047141
6	5.280476	2.669334	-1.559948
6	5.527998	1.290746	-1.587644
1	6.485922	0.908251	-1.949512
1	6.040808	3.367268	-1.918424
1	3.893334	4.235035	-0.998761
1	2.168927	2.691777	-0.146840

**Cam-B3LYP(D3)/ 6-311+g\*\*/meta-stable product/C-PCM(ACN)**

6	-1.327196	0.487886	0.141660
6	-0.074624	-0.379602	0.422592
6	1.085218	0.667077	0.507974
6	-0.864024	1.854837	-0.094328
6	0.393795	4.332026	-0.192744
6	0.505887	1.962628	0.182316
6	1.106427	3.226272	0.224533
1	2.125902	3.335947	0.566315
6	-2.625001	0.075718	0.195167
6	-3.187724	-1.285978	-0.046072
6	-3.821822	0.927889	0.467688
6	-2.601637	-2.514944	-0.343079
6	-4.594342	-1.197006	-0.069145
6	-3.942808	2.191230	1.043244
6	-4.985920	0.162936	0.288514
6	-3.403149	-3.614004	-0.632845
1	-1.532536	-2.645013	-0.355044
6	-5.393102	-2.289351	-0.369425
6	-5.202831	2.706367	1.319868
1	-3.072827	2.780239	1.292830

6	-6.247400	0.677943	0.553084
6	-4.789754	-3.508014	-0.650083
1	-2.933872	-4.566072	-0.850233
1	-6.472575	-2.194801	-0.385503
6	-6.353528	1.968061	1.052827
1	-5.287261	3.693531	1.758250
1	-7.134033	0.073140	0.402801
1	-5.397177	-4.374284	-0.882972
1	-7.328387	2.388552	1.268404
1	0.856983	5.310963	-0.175662
6	2.430269	0.430744	0.618713
6	3.154553	-0.587550	1.415312
6	3.487523	1.073615	-0.222349
6	2.777046	-1.325320	2.536777
6	4.516253	-0.581294	1.053110
6	3.414714	1.963655	-1.295325
6	4.711394	0.415459	0.007719
6	3.708395	-2.128729	3.183728
1	1.782505	-1.259068	2.943548
6	5.448370	-1.379387	1.699760
6	4.550777	2.246268	-2.041513
1	2.487082	2.443298	-1.568019
6	5.848339	0.697749	-0.738141
6	5.032878	-2.177036	2.757421
1	3.399496	-2.709262	4.044844
1	6.490466	-1.363292	1.402348
6	5.769751	1.633380	-1.758228
1	4.482007	2.951720	-2.861108
1	6.778553	0.177532	-0.541108
1	5.745922	-2.807288	3.275128
1	6.646064	1.869514	-2.349745
6	-0.913598	4.187349	-0.668440
1	-1.443515	5.047431	-1.059222
6	-1.546411	2.960914	-0.611406
1	-2.564740	2.867558	-0.957792
6	-0.343100	-1.177683	1.709549
1	-1.331254	-1.628024	1.681913
1	0.373019	-1.976261	1.862790
1	-0.310392	-0.510488	2.571910
6	0.308945	-1.245335	-0.796177
6	1.063631	-2.410098	-0.659322
6	-0.039594	-0.839214	-2.083904
6	1.439368	-3.153026	-1.771258
1	1.367954	-2.758165	0.317812
6	0.337478	-1.577888	-3.197589
1	-0.624156	0.060934	-2.227315
6	1.077254	-2.742543	-3.047002
1	2.018222	-4.058990	-1.635250
1	0.046153	-1.241267	-4.185569
1	1.368189	-3.324094	-3.913443

**Cam-B3LYP(D3)/ 6-311+g\*\*/meta-stable product/C-PCM(CHX)**

6	-1.326629	0.485319	0.126938
6	-0.075508	-0.384985	0.398769
6	1.087158	0.658307	0.484266
6	-0.859772	1.848784	-0.120529
6	0.406325	4.318812	-0.256075
6	0.513029	1.952871	0.142763
6	1.118333	3.214820	0.166022
1	2.141237	3.323262	0.497505
6	-2.625402	0.078913	0.192323
6	-3.196524	-1.279456	-0.044834
6	-3.814274	0.936237	0.480860

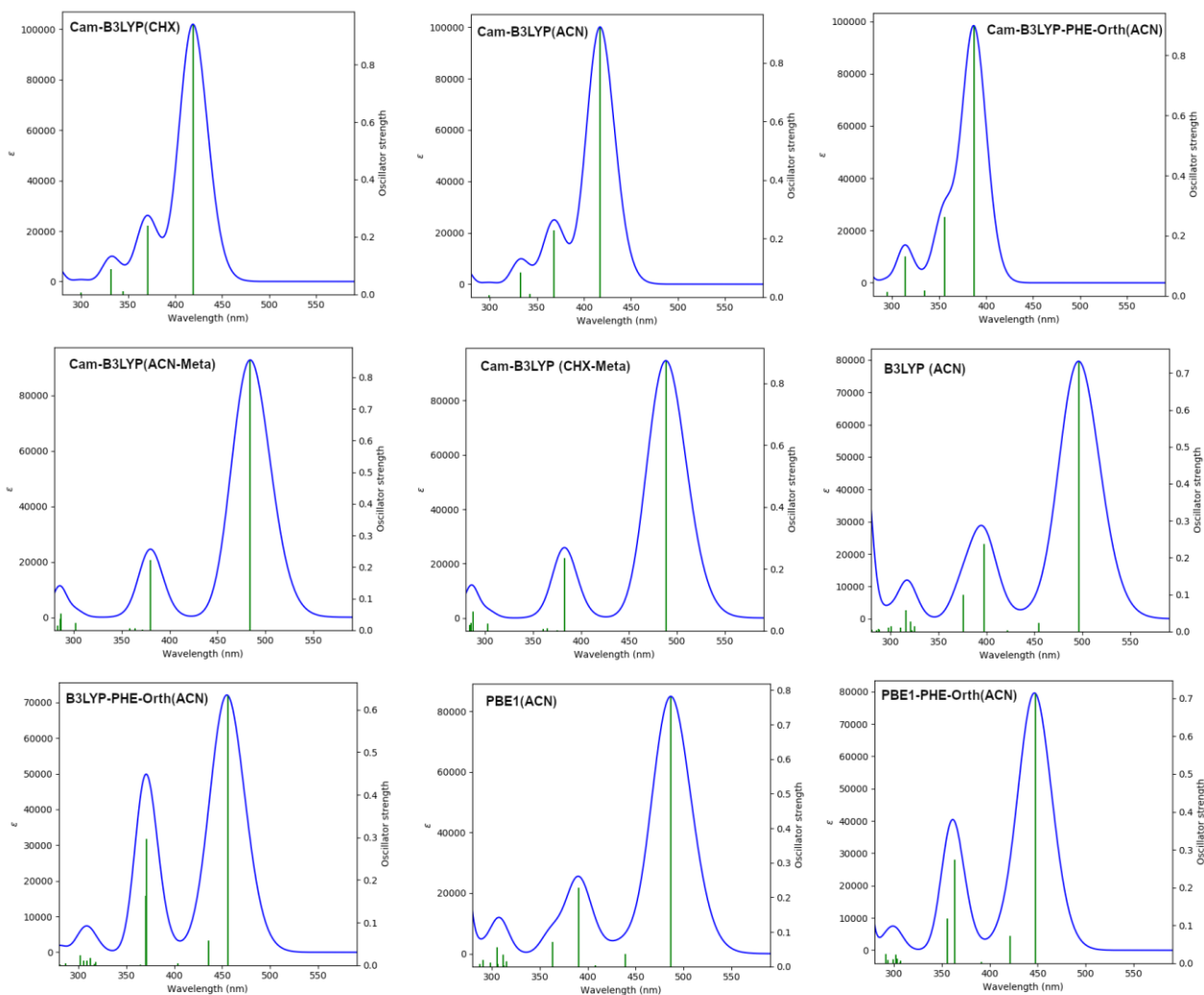


6	-2.618477	-2.506730	-0.362392
6	-4.602565	-1.185792	-0.043231
6	-3.920655	2.200623	1.056018
6	-4.983419	0.175170	0.321642
6	-3.427810	-3.601728	-0.643152
1	-1.549883	-2.637178	-0.400799
6	-5.408648	-2.274487	-0.334295
6	-5.173596	2.721229	1.352077
1	-3.043456	2.785165	1.290806
6	-6.237534	0.695959	0.606378
6	-4.813669	-3.492686	-0.632110
1	-2.964767	-4.552585	-0.878169
1	-6.487986	-2.177011	-0.331645
6	-6.330687	1.986841	1.105485
1	-5.247307	3.709118	1.790840
1	-7.128871	0.094362	0.471996
1	-5.427376	-4.356211	-0.858808
1	-7.300301	2.411146	1.336782
1	0.874313	5.295761	-0.253443
6	2.430151	0.420568	0.611084
6	3.147188	-0.582299	1.433971
6	3.495904	1.051966	-0.226836
6	2.758651	-1.302019	2.563001
6	4.513556	-0.574731	1.091016
6	3.431228	1.918415	-1.318682
6	4.718987	0.404984	0.031949
6	3.684514	-2.089150	3.236635
1	1.758373	-1.232856	2.954749
6	5.439734	-1.356305	1.764495
6	4.575260	2.194295	-2.054067
1	2.502502	2.381733	-1.615161
6	5.863555	0.679924	-0.703693
6	5.014371	-2.137794	2.829595
1	3.367040	-2.655310	4.104242
1	6.485807	-1.338638	1.481564
6	5.793557	1.595589	-1.741671
1	4.513191	2.881166	-2.889806
1	6.793558	0.167968	-0.485298
1	5.723541	-2.754691	3.368307
1	6.676337	1.825361	-2.326048
6	-0.906625	4.175709	-0.716212
1	-1.436962	5.034192	-1.110280
6	-1.543485	2.952789	-0.640438
1	-2.566207	2.858506	-0.973906
6	-0.339525	-1.194265	1.679181
1	-1.323309	-1.653570	1.646263
1	0.385392	-1.986275	1.826886
1	-0.315896	-0.532319	2.546082
6	0.303192	-1.246242	-0.824854
6	1.094369	-2.387332	-0.695330
6	-0.086359	-0.862215	-2.106732
6	1.464727	-3.129626	-1.808443
1	1.437283	-2.712006	0.277187
6	0.285247	-1.600929	-3.221851
1	-0.701036	0.018567	-2.243148
6	1.060456	-2.742170	-3.078426
1	2.075436	-4.015308	-1.678460
1	-0.038821	-1.282399	-4.205566
1	1.348187	-3.323053	-3.946367

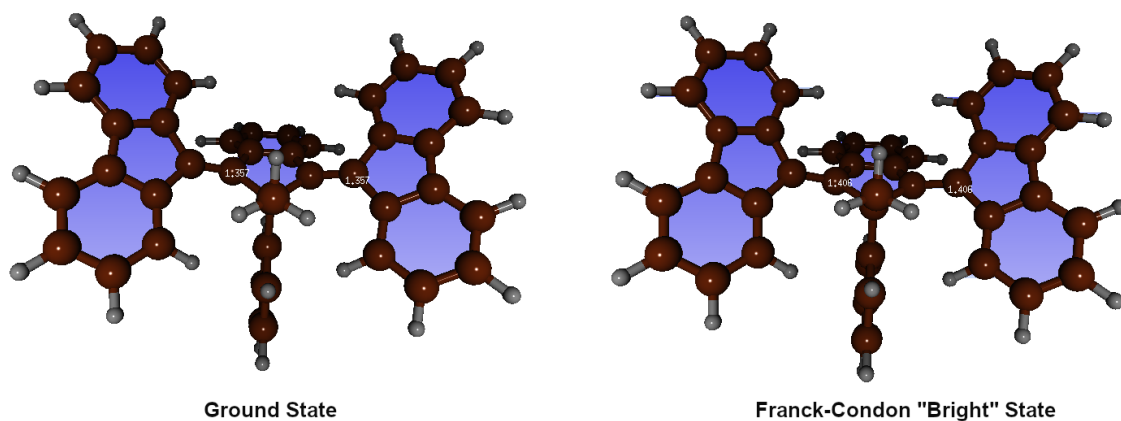
Cam-B3LYP(D3)/6-311+g\*\*/Excited State/C-PCM(ACN)

6	1.194971	0.205481	0.354773
6	-0.000120	-0.732442	0.052082
6	-1.194978	0.205860	0.354544
6	0.723033	1.137207	1.292295
6	-0.713914	2.684438	3.126653
6	-0.722993	1.137651	1.291881
6	-1.421218	1.930503	2.236267
1	-2.501930	1.904030	2.270624
6	2.474556	0.188498	-0.233347
6	3.251952	-0.917141	-0.792624
6	3.290212	1.386228	-0.428725
6	2.997976	-2.286900	-0.940864
6	4.515640	-0.421345	-1.211556
6	2.995634	2.746569	-0.281554
6	4.533387	1.017736	-0.997653
6	3.968628	-3.115451	-1.485864
1	2.057697	-2.722559	-0.644964
6	5.482313	-1.254019	-1.745586
6	3.953295	3.693836	-0.615706
1	2.029372	3.073373	0.074632
6	5.487555	1.965428	-1.322643
6	5.206155	-2.611146	-1.883340
1	3.757176	-4.171717	-1.601181
1	6.441287	-0.855260	-2.055849
6	5.199243	3.311942	-1.114335
1	3.723815	4.745815	-0.495312
1	6.437571	1.668692	-1.751998
1	5.951915	-3.276136	-2.301844
1	5.934631	4.067063	-1.364514
1	-1.237358	3.271737	3.871101
6	-2.474608	0.188858	-0.233455
6	-3.290011	1.386571	-0.429420
6	-3.252225	-0.917009	-0.791796
6	-2.995289	2.746878	-0.282298
6	-4.533028	1.018070	-0.998714
6	-2.998664	-2.287025	-0.938286
6	-4.515575	-0.421168	-1.211701
6	-3.952637	3.694211	-0.617158
1	-2.029162	3.073554	0.074418
6	-5.486851	1.965851	-1.324448
6	-3.969347	-3.115793	-1.482897
1	-2.058732	-2.722668	-0.641205
6	-5.482263	-1.254060	-1.745362
6	-5.198373	3.312380	-1.116392
1	-3.723083	4.746184	-0.496847
1	-6.436759	1.669167	-1.754079
6	-5.206467	-2.611425	-1.881603
1	-3.758274	-4.172277	-1.596905
1	-6.441000	-0.855331	-2.056394
1	-5.933515	4.067560	-1.367114
1	-5.952259	-3.276592	-2.299768
6	0.713745	2.683829	3.127224
1	1.237091	3.270692	3.872084
6	1.421135	1.929391	2.237318
1	2.501797	1.902144	2.272461
6	-0.000097	-1.301853	-1.382687
1	0.000766	-2.390214	-1.397816
1	-0.875061	-0.963746	-1.932461
1	0.873927	-0.962290	-1.933053
6	-0.000182	-1.810995	1.185875
6	-1.191280	-2.282401	1.741113

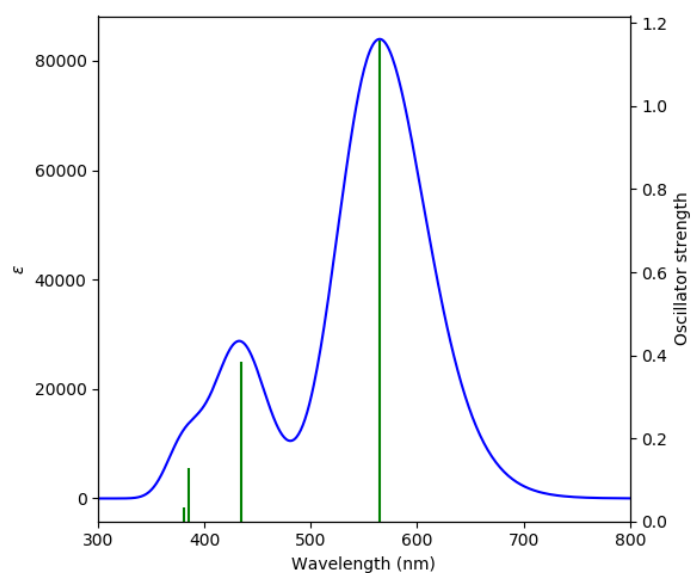
6	1.191006	-2.283819	1.739671
6	-1.194362	-3.233224	2.753419
1	-2.141309	-1.893130	1.410855
6	1.194191	-3.234632	2.751979
1	2.141064	-1.895410	1.408525
6	-0.000073	-3.726063	3.258040
1	-2.140499	-3.575818	3.155406
1	2.140408	-3.578262	3.152896
1	-0.000031	-4.465642	4.049590



**Figure S1:** UV/Vis absorption spectra and oscillator strength in ACN and CHX at C-PCM/[B3LYP(D3), Cam-B3LYP(D3) and PBE1PBE(D3)]/6-311+G\*\* level for the two PHE-based rotamer of the simulated motor. The label PHE-Orth refers to the rotamer with the aromatic ring featuring an orthogonal mutual orientation with respect to the rotating arm (see Fig. 2, right panel in the manuscript). The absorption spectra of the metastable form (see Fig. 1, right panel) in ACN and CHX solution is also reported at C-PCM/Cam-B3LYP(D3)/6-311+G\*\* level.



**Figure S2:** Optimized geometries at Cam-B3LYP(D3)/6-311G\*\*//C-PCM (ACN) level of theory. In this picture is also reported the elongation of the rotational axes when passing from ground-state to Frank-Condon "Bright" state.



**Figure S3:** Fluorescence spectrum of the investigated molecular rotor in acetonitrile dilute solution at Cam-B3LYP(D3)/6-311G\*\*//C-PCM level of theory. Oscillator strengths are also reported as green histograms.

### Topology file (Acetonitrile, ACN)

; This include topology was generated for the paper below:  
 ; Carl Caleman, Paul J. van Maaren, Minyan Hong, Jochen S. Hub,  
 ; Luciano T. Costa and David van der Spoel  
 ; Force Field Benchmark of Organic Liquids: Density,  
 ; Enthalpy of Vaporization, Heat Capacities, Surface Tension,  
 ; Isothermal Compressibility, Volumetric Expansion Coefficient,  
 ; and Dielectric Constant

; J. Chem. Theor. Comput. 8 (2012) 61-74  
; http://dx.doi.org/10.1021/ct200731v  
; REFERENCE Caleman2012a  
; Corrected nrexcl to 3. DvdS, 2011-09-12

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[ moleculetype ]
; Name      nrexcl
ACN         3

[ atoms ]
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  3  opls_759  1  ACN   H   1    0.06   1.0079 ;qtot 0
  4  opls_759  1  ACN   H   1    0.06   1.0079 ;qtot 0
  5  opls_754  1  ACN   C   2    0.46    0 ;qtot 0
  6  opls_753  1  ACN   N   3   -0.56    0 ;qtot 0
  7    ML    1  ACN   ML   4    0  24.1707 ;qtot 0

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; ai  aj funct      c0      c1      c2      c3
  1  2  1  0.10900  284512.0
  1  3  1  0.10900  284512.0
  1  4  1  0.10900  284512.0

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  1  7  1  2.232581e-01  1e7
#else
[ constraints ]
; ai  aj funct      c0      c1
  1  7  1  2.232581e-01  0.000000e+00
#endif

[ exclusions ]
; i  excluded from i
  1  2  3  4  5
  2  1
  3  1
  4  1
  5  1  6  2  3  4
  6  6  5  1
  7  7

[ angles ]
; ai  aj  ak funct      c0      c1      c2      c3
  2  1  3  1      107.800  276.144 ; HC - CT - HC
  2  1  4  1      107.800  276.144 ; HC - CT - HC
  2  1  5  1      110.700  313.800 ; CT - CT - HC
  3  1  4  1      107.800  276.144 ; HC - CT - HC
  3  1  5  1      110.700  313.800 ; CT - CT - HC
  4  1  5  1      110.700  313.800 ; CT - CT - HC

[ virtual_sites2 ]
; ai  aj  ak funct      c0
  5  1  7  1  6.517123e-01
  6  1  7  1  1.166811e+00
```

### Gro-coordinates file (Molecular rotor, most stable rotamer)

LIGPARGEN GENERATED GRO FILE  
70

1GMR	C00	1	0.100	0.100	0.000
1GMR	C01	2	-0.056	0.100	0.000
1GMR	C02	3	-0.085	0.100	0.153
1GMR	C03	4	0.034	0.155	0.218
1GMR	C04	5	0.141	0.155	0.129
1GMR	C05	6	0.258	0.224	0.160
1GMR	C06	7	0.267	0.290	0.282
1GMR	C07	8	0.161	0.287	0.372
1GMR	C08	9	0.043	0.224	0.339
1GMR	C09	10	-0.107	-0.031	-0.062
1GMR	H0A	11	0.339	0.230	0.089
1GMR	H0B	12	0.356	0.348	0.305
1GMR	H0C	13	0.170	0.338	0.467
1GMR	H0D	14	-0.043	0.233	0.404
1GMR	C0E	15	-0.111	0.228	-0.066
1GMR	H0F	16	-0.062	-0.114	-0.008
1GMR	H0G	17	-0.079	-0.040	-0.166
1GMR	H0H	18	-0.215	-0.040	-0.054
1GMR	C0I	19	-0.200	0.223	-0.174
1GMR	C0J	20	-0.248	0.339	-0.233
1GMR	C0K	21	-0.210	0.463	-0.185
1GMR	C0M	22	-0.121	0.470	-0.078
1GMR	C0N	23	-0.072	0.354	-0.020
1GMR	H0O	24	-0.232	0.127	-0.213
1GMR	H0P	25	-0.317	0.331	-0.316
1GMR	H0Q	26	-0.248	0.553	-0.231
1GMR	H0R	27	-0.090	0.566	-0.039
1GMR	H0S	28	-0.003	0.362	0.063
1GMR	C0T	29	-0.194	0.052	0.219
1GMR	C0U	30	-0.193	-0.005	0.357
1GMR	C0V	31	-0.322	-0.049	0.389
1GMR	C0W	32	-0.411	-0.017	0.278
1GMR	C0X	33	-0.335	0.039	0.174
1GMR	C0Y	34	-0.400	0.084	0.060
1GMR	C0Z	35	-0.537	0.068	0.048
1GMR	C10	36	-0.611	0.005	0.148
1GMR	C11	37	-0.548	-0.035	0.266
1GMR	H12	38	-0.717	-0.012	0.135
1GMR	H13	39	-0.587	0.104	-0.042
1GMR	H14	40	-0.605	-0.080	0.347
1GMR	H15	41	-0.346	0.133	-0.020
1GMR	C16	42	-0.088	-0.036	0.444
1GMR	C17	43	-0.115	-0.103	0.562
1GMR	C18	44	-0.245	-0.139	0.597
1GMR	C19	45	-0.349	-0.117	0.508
1GMR	H1A	46	0.014	-0.009	0.420
1GMR	H1B	47	-0.033	-0.127	0.629
1GMR	H1C	48	-0.265	-0.185	0.693
1GMR	H1D	49	-0.450	-0.151	0.530
1GMR	C1E	50	0.185	0.052	-0.095
1GMR	C1F	51	0.320	-0.005	-0.068
1GMR	C1G	52	0.166	0.039	-0.241
1GMR	C1H	53	0.376	-0.049	-0.189
1GMR	C1I	54	0.283	-0.017	-0.297
1GMR	C1J	55	0.497	-0.117	-0.193
1GMR	C1K	56	0.564	-0.142	-0.074
1GMR	C1M	57	0.510	-0.098	0.046
1GMR	C1N	58	0.386	-0.036	0.051
1GMR	H1O	59	0.658	-0.195	-0.076
1GMR	H1P	60	0.565	-0.112	0.138
1GMR	H1Q	61	0.342	-0.013	0.147
1GMR	H1R	62	0.538	-0.151	-0.288
1GMR	C1S	63	0.066	0.084	-0.327
1GMR	C1T	64	0.080	0.067	-0.464

1GMR C1U 65 0.193 0.006 -0.518  
1GMR C1V 66 0.297 -0.033 -0.434  
1GMR H1W 67 0.388 -0.075 -0.476  
1GMR H1X 68 0.199 -0.012 -0.624  
1GMR H1Y 69 0.001 0.103 -0.530  
1GMR H1Z 70 -0.022 0.132 -0.288

### Topology file (Molecular rotor, most stable rotamer)

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;  
; GENERATED BY LigParGen Server  
; Jorgensen Lab @ Yale University  
;  
[ atomtypes ]  
opls_863 C863 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_854 C854 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_826 H826 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_829 C829 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_859 H859 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_858 H858 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_856 C856 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_830 C830 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_855 C855 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_835 C835 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_865 C865 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_844 C844 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_846 H846 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_862 C862 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_843 C843 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_823 H823 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_868 H868 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_814 C814 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_864 C864 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_833 C833 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_852 C852 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_866 H866 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_815 H815 1.0080 0.000 A 2.50000E-01 1.25520E-01  
opls_801 C801 12.0110 0.000 A 3.50000E-01 2.76144E-01  
opls_841 C841 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_837 H837 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_818 C818 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_840 H840 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_832 C832 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_821 C821 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_812 H812 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_847 H847 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_819 C819 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_869 H869 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_805 C805 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_803 C803 12.0110 0.000 A 3.55000E-01 3.17984E-01  
opls_845 H845 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_816 H816 1.0080 0.000 A 2.50000E-01 1.25520E-01  
opls_811 H811 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_867 H867 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_810 H810 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_802 C802 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_804 C804 12.0110 0.000 A 3.55000E-01 3.17984E-01  
opls_827 H827 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_834 C834 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_824 H824 1.0080 0.000 A 2.42000E-01 1.25520E-01  
opls_806 C806 12.0110 0.000 A 3.55000E-01 2.92880E-01  
opls_828 C828 12.0110 0.000 A 3.55000E-01 3.17984E-01
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opls_800 C800 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_849 C849 12.0110 0.000 A 3.55000E-01 3.17984E-01
opls_857 C857 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_853 C853 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_861 H861 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_813 H813 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_809 C809 12.0110 0.000 A 3.50000E-01 2.76144E-01
opls_807 C807 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_825 H825 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_817 H817 1.0080 0.000 A 2.50000E-01 1.25520E-01
opls_820 C820 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_839 H839 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_822 C822 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_850 C850 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_860 H860 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_851 C851 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_836 C836 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_848 H848 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_808 C808 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_838 H838 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_831 C831 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_842 C842 12.0110 0.000 A 3.55000E-01 2.92880E-01

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[ moleculetype ]

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; Name nrexcl
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GMR 3
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[ atoms ]

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; nr type resnr residue atom cgnr charge mass
 1 opls_800 1 GMR C00 1 -0.022 12.0110
 2 opls_801 1 GMR C01 1 0.0841 12.0110
 3 opls_802 1 GMR C02 1 -0.0221 12.0110
 4 opls_803 1 GMR C03 1 -0.0555 12.0110
 5 opls_804 1 GMR C04 1 -0.0547 12.0110
 6 opls_805 1 GMR C05 1 -0.1109 12.0110
 7 opls_806 1 GMR C06 1 -0.1353 12.0110
 8 opls_807 1 GMR C07 1 -0.1351 12.0110
 9 opls_808 1 GMR C08 1 -0.1101 12.0110
10 opls_809 1 GMR C09 1 -0.239 12.0110
11 opls_810 1 GMR HOA 1 0.1586 1.0080
12 opls_811 1 GMR HOB 1 0.1437 1.0080
13 opls_812 1 GMR HOC 1 0.1437 1.0080
14 opls_813 1 GMR HOD 1 0.1577 1.0080
15 opls_814 1 GMR COE 1 -0.0666 12.0110
16 opls_815 1 GMR HOF 1 0.1036 1.0080
17 opls_816 1 GMR HOG 1 0.1036 1.0080
18 opls_817 1 GMR HOH 1 0.1036 1.0080
19 opls_818 1 GMR COI 1 -0.1474 12.0110
20 opls_819 1 GMR COJ 1 -0.1394 12.0110
21 opls_820 1 GMR COK 1 -0.1314 12.0110
22 opls_821 1 GMR COM 1 -0.1325 12.0110
23 opls_822 1 GMR CON 1 -0.1176 12.0110
24 opls_823 1 GMR HOO 1 0.1412 1.0080
25 opls_824 1 GMR HOP 1 0.1385 1.0080
26 opls_825 1 GMR HOQ 1 0.1406 1.0080
27 opls_826 1 GMR HOR 1 0.1401 1.0080
28 opls_827 1 GMR HOS 1 0.1505 1.0080
29 opls_828 1 GMR COT 1 -0.0094 12.0110
30 opls_829 1 GMR COU 1 -0.0523 12.0110
31 opls_830 1 GMR COV 1 -0.0466 12.0110
32 opls_831 1 GMR COW 1 -0.0446 12.0110
33 opls_832 1 GMR COX 2 -0.0453 12.0110
34 opls_833 1 GMR COY 2 -0.1132 12.0110
35 opls_834 1 GMR COZ 2 -0.1398 12.0110
36 opls_835 1 GMR C10 2 -0.1327 12.0110
37 opls_836 1 GMR C11 2 -0.1112 12.0110

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38	opls_837	1	GMR	H12	2	0.1392	1.0080
39	opls_838	1	GMR	H13	2	0.1386	1.0080
40	opls_839	1	GMR	H14	2	0.1428	1.0080
41	opls_840	1	GMR	H15	2	0.1537	1.0080
42	opls_841	1	GMR	C16	2	-0.1113	12.0110
43	opls_842	1	GMR	C17	2	-0.1397	12.0110
44	opls_843	1	GMR	C18	2	-0.1339	12.0110
45	opls_844	1	GMR	C19	2	-0.1099	12.0110
46	opls_845	1	GMR	H1A	2	0.15	1.0080
47	opls_846	1	GMR	H1B	2	0.1388	1.0080
48	opls_847	1	GMR	H1C	2	0.1396	1.0080
49	opls_848	1	GMR	H1D	2	0.1424	1.0080
50	opls_849	1	GMR	C1E	2	-0.0097	12.0110
51	opls_850	1	GMR	C1F	2	-0.0527	12.0110
52	opls_851	1	GMR	C1G	2	-0.0454	12.0110
53	opls_852	1	GMR	C1H	2	-0.046	12.0110
54	opls_853	1	GMR	C1I	2	-0.0446	12.0110
55	opls_854	1	GMR	C1J	2	-0.1105	12.0110
56	opls_855	1	GMR	C1K	2	-0.1332	12.0110
57	opls_856	1	GMR	C1M	2	-0.1399	12.0110
58	opls_857	1	GMR	C1N	2	-0.1109	12.0110
59	opls_858	1	GMR	H1O	2	0.1399	1.0080
60	opls_859	1	GMR	H1P	2	0.1381	1.0080
61	opls_860	1	GMR	H1Q	2	0.1503	1.0080
62	opls_861	1	GMR	H1R	2	0.1423	1.0080
63	opls_862	1	GMR	C1S	2	-0.1136	12.0110
64	opls_863	1	GMR	C1T	2	-0.1398	12.0110
65	opls_864	1	GMR	C1U	2	-0.1326	12.0110
66	opls_865	1	GMR	C1V	3	-0.1109	12.0110
67	opls_866	1	GMR	H1W	3	0.1425	1.0080
68	opls_867	1	GMR	H1X	3	0.1392	1.0080
69	opls_868	1	GMR	H1Y	3	0.1386	1.0080
70	opls_869	1	GMR	H1Z	3	0.1537	1.0080

[ bonds ]

2	1	1	0.1495	265265.600
3	2	1	0.1495	265265.600
4	3	1	0.1433	357313.600
5	1	1	0.1433	357313.600
6	5	1	0.1433	357313.600
7	6	1	0.1400	392459.200
8	7	1	0.1400	392459.200
9	4	1	0.1433	357313.600
10	2	1	0.1529	224262.400
11	6	1	0.1080	307105.600
12	7	1	0.1080	307105.600
13	8	1	0.1080	307105.600
14	9	1	0.1080	307105.600
15	2	1	0.1510	265265.600
16	10	1	0.1090	284512.000
17	10	1	0.1090	284512.000
18	10	1	0.1090	284512.000
19	15	1	0.1400	392459.200
20	19	1	0.1400	392459.200
21	20	1	0.1400	392459.200
22	21	1	0.1400	392459.200
23	15	1	0.1400	392459.200
24	19	1	0.1080	307105.600
25	20	1	0.1080	307105.600
26	21	1	0.1080	307105.600
27	22	1	0.1080	307105.600
28	23	1	0.1080	307105.600
29	3	1	0.1433	357313.600
30	29	1	0.1433	357313.600
31	30	1	0.1424	392459.200

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32 31 1 0.1424 392459.200
33 29 1 0.1433 357313.600
34 33 1 0.1400 392459.200
35 34 1 0.1400 392459.200
36 35 1 0.1400 392459.200
37 32 1 0.1400 392459.200
38 36 1 0.1080 307105.600
39 35 1 0.1080 307105.600
40 37 1 0.1080 307105.600
41 34 1 0.1080 307105.600
42 30 1 0.1400 392459.200
43 42 1 0.1400 392459.200
44 43 1 0.1400 392459.200
45 31 1 0.1400 392459.200
46 42 1 0.1080 307105.600
47 43 1 0.1080 307105.600
48 44 1 0.1080 307105.600
49 45 1 0.1080 307105.600
50 1 1 0.1433 357313.600
51 50 1 0.1433 357313.600
52 50 1 0.1433 357313.600
53 51 1 0.1424 392459.200
54 52 1 0.1424 392459.200
55 53 1 0.1400 392459.200
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62 55 1 0.1080 307105.600
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65 64 1 0.1400 392459.200
66 54 1 0.1400 392459.200
67 66 1 0.1080 307105.600
68 65 1 0.1080 307105.600
69 64 1 0.1080 307105.600
70 63 1 0.1080 307105.600
5 4 1 0.1460 322168.000
9 8 1 0.1400 392459.200
23 22 1 0.1400 392459.200
33 32 1 0.1424 392459.200
37 36 1 0.1400 392459.200
45 44 1 0.1400 392459.200
54 53 1 0.1424 392459.200
58 57 1 0.1400 392459.200
66 65 1 0.1400 392459.200

```

[ angles ]

```

; ai aj ak funct c0 c1 c2 c3
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2 3 4 1 119.200 525.092
2 1 5 1 119.200 525.092
1 5 6 1 115.690 382.752
5 6 7 1 124.000 585.760
6 7 8 1 120.000 527.184
3 4 9 1 115.690 382.752
1 2 10 1 115.600 527.184
5 6 11 1 118.990 539.820
6 7 12 1 120.000 292.880
7 8 13 1 120.000 292.880
4 9 14 1 118.990 539.820
1 2 15 1 109.500 334.720
2 10 16 1 110.700 313.800

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2	10	17	1	110.700	313.800
2	10	18	1	110.700	313.800
2	15	19	1	120.000	585.760
15	19	20	1	120.000	527.184
19	20	21	1	120.000	527.184
20	21	22	1	120.000	527.184
2	15	23	1	120.000	585.760
15	19	24	1	120.000	292.880
19	20	25	1	120.000	292.880
20	21	26	1	120.000	292.880
21	22	27	1	120.000	292.880
15	23	28	1	120.000	292.880
2	3	29	1	119.200	525.092
3	29	30	1	115.690	382.752
29	30	31	1	124.000	585.760
30	31	32	1	120.000	527.184
3	29	33	1	115.690	382.752
29	33	34	1	124.000	585.760
33	34	35	1	120.000	527.184
34	35	36	1	120.000	527.184
31	32	37	1	120.000	527.184
35	36	38	1	120.000	292.880
34	35	39	1	120.000	292.880
32	37	40	1	120.000	292.880
33	34	41	1	120.000	292.880
29	30	42	1	124.000	585.760
30	42	43	1	120.000	527.184
42	43	44	1	120.000	527.184
30	31	45	1	120.000	527.184
30	42	46	1	120.000	292.880
42	43	47	1	120.000	292.880
43	44	48	1	120.000	292.880
31	45	49	1	120.000	292.880
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1	50	52	1	115.690	382.752
50	51	53	1	124.000	585.760
50	52	54	1	124.000	585.760
51	53	55	1	120.000	527.184
53	55	56	1	120.000	527.184
55	56	57	1	120.000	527.184
50	51	58	1	124.000	585.760
55	56	59	1	120.000	292.880
56	57	60	1	120.000	292.880
51	58	61	1	120.000	292.880
53	55	62	1	120.000	292.880
50	52	63	1	124.000	585.760
52	63	64	1	120.000	527.184
63	64	65	1	120.000	527.184
52	54	66	1	120.000	527.184
54	66	67	1	120.000	292.880
64	65	68	1	120.000	292.880
63	64	69	1	120.000	292.880
52	63	70	1	120.000	292.880
56	55	62	1	120.000	292.880
66	65	68	1	120.000	292.880
65	64	69	1	120.000	292.880
8	7	12	1	120.000	292.880
20	19	24	1	120.000	292.880
54	53	55	1	120.000	527.184
57	56	59	1	120.000	292.880
45	44	48	1	120.000	292.880
53	51	58	1	120.000	527.184
32	37	36	1	120.000	527.184

```

19 15 23 1 120.000 527.184
51 50 52 1 115.690 382.752
64 63 70 1 120.000 292.880
3 2 10 1 115.600 527.184
36 37 40 1 120.000 292.880
56 57 58 1 120.000 527.184
3 2 15 1 109.500 334.720
5 4 9 1 117.000 711.280
53 54 66 1 120.000 527.184
44 45 49 1 120.000 292.880
37 36 38 1 120.000 292.880
22 23 28 1 120.000 292.880
30 29 33 1 115.690 382.752
57 58 61 1 120.000 292.880
4 3 29 1 119.200 525.092
58 57 60 1 120.000 292.880
10 2 15 1 114.000 527.184
32 33 34 1 120.000 527.184
52 54 53 1 120.000 527.184
21 22 23 1 120.000 527.184
8 9 14 1 120.000 292.880
54 52 63 1 120.000 527.184
16 10 17 1 107.800 276.144
35 34 41 1 120.000 292.880
54 66 65 1 120.000 527.184
5 1 50 1 119.200 525.092
4 9 8 1 124.000 585.760
43 42 46 1 120.000 292.880
7 6 11 1 120.000 292.880
16 10 18 1 107.800 276.144
35 36 37 1 120.000 527.184
36 35 39 1 120.000 292.880
32 31 45 1 120.000 527.184
17 10 18 1 107.800 276.144
22 21 26 1 120.000 292.880
15 23 22 1 120.000 527.184
7 8 9 1 120.000 527.184
23 22 27 1 120.000 292.880
3 4 5 1 117.000 711.280
33 32 37 1 120.000 527.184
4 5 6 1 117.000 711.280
1 5 4 1 117.000 711.280
65 66 67 1 120.000 292.880
29 33 32 1 124.000 585.760
43 44 45 1 120.000 527.184
9 8 13 1 120.000 292.880
44 43 47 1 120.000 292.880
31 45 44 1 120.000 527.184
64 65 66 1 120.000 527.184
51 53 54 1 120.000 527.184
31 32 33 1 120.000 527.184
21 20 25 1 120.000 292.880
31 30 42 1 120.000 527.184
51 58 57 1 120.000 527.184

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[ dihedrals ]

; IMPROPER DIHEDRAL ANGLES

```

; ai aj ak al funct c0 c1 c2 c3 c4 c5
50 1 2 5 4 180.000 10.460 2
29 3 2 4 4 180.000 10.460 2
6 5 1 4 4 180.000 10.460 2
9 4 3 5 4 180.000 10.460 2
23 15 2 19 4 180.000 10.460 2
34 33 29 32 4 180.000 10.460 2

```

42	30	29	31	4	180.000	10.460	2
58	51	50	53	4	180.000	10.460	2
63	52	50	54	4	180.000	10.460	2
55	53	51	54	4	180.000	10.460	2
37	32	31	33	4	180.000	10.460	2
66	54	52	53	4	180.000	10.460	2
45	31	30	32	4	180.000	10.460	2
33	29	3	30	4	180.000	10.460	2
52	50	1	51	4	180.000	10.460	2
11	6	5	7	4	180.000	10.460	2
14	9	4	8	4	180.000	10.460	2
27	22	21	23	4	180.000	10.460	2
38	36	35	37	4	180.000	10.460	2
26	21	20	22	4	180.000	10.460	2
69	64	63	65	4	180.000	10.460	2
68	65	64	66	4	180.000	10.460	2
24	19	15	20	4	180.000	10.460	2
25	20	19	21	4	180.000	10.460	2
28	23	15	22	4	180.000	10.460	2
12	7	6	8	4	180.000	10.460	2
60	57	56	58	4	180.000	10.460	2
59	56	55	57	4	180.000	10.460	2
47	43	42	44	4	180.000	10.460	2
13	8	7	9	4	180.000	10.460	2
48	44	43	45	4	180.000	10.460	2
39	35	34	36	4	180.000	10.460	2
46	42	30	43	4	180.000	10.460	2
40	37	32	36	4	180.000	10.460	2
70	63	52	64	4	180.000	10.460	2
61	58	51	57	4	180.000	10.460	2
62	55	53	56	4	180.000	10.460	2
67	66	54	65	4	180.000	10.460	2
49	45	31	44	4	180.000	10.460	2
41	34	33	35	4	180.000	10.460	2

[ dihedrals ]

; PROPER DIHEDRAL ANGLES

; ai	aj	ak	al	funct	c0	c1	c2	c3	c4	c5
5	4	3	2	3	0.527	-6.397	-1.695	7.565	-0.000	0.000
4	5	1	2	3	0.527	-6.397	-1.695	7.565	-0.000	0.000
50	1	5	4	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
29	3	4	5	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
29	3	4	9	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
50	1	5	6	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
29	3	2	15	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
50	1	2	15	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
4	3	2	1	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
50	1	2	3	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
29	3	2	1	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
5	1	2	3	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
29	3	2	10	3	0.000	0.000	0.000	-0.000	-0.000	0.000
50	1	2	10	3	0.000	0.000	0.000	-0.000	-0.000	0.000
9	4	5	6	3	0.628	1.883	0.000	-2.510	-0.000	0.000
9	4	5	1	3	0.628	1.883	0.000	-2.510	-0.000	0.000
6	5	4	3	3	0.628	1.883	0.000	-2.510	-0.000	0.000
9	4	3	2	3	58.576	0.000	-58.576	-0.000	-0.000	0.000
6	5	1	2	3	58.576	0.000	-58.576	-0.000	-0.000	0.000
7	6	5	4	3	16.027	-4.391	-14.029	2.393	-0.000	0.000
8	9	4	5	3	16.027	-4.391	-14.029	2.393	-0.000	0.000
7	6	5	1	3	16.027	-4.391	-14.029	2.393	-0.000	0.000
8	9	4	3	3	16.027	-4.391	-14.029	2.393	-0.000	0.000
7	8	9	4	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
8	7	6	5	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
23	22	21	20	3	30.334	0.000	-30.334	-0.000	-0.000	0.000

21	20	19	15	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
22	21	20	19	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
66	65	64	63	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
22	23	15	19	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
37	36	35	34	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
21	22	23	15	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
58	57	56	55	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
45	44	43	42	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
9	8	7	6	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
23	15	19	20	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
65	64	63	52	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
56	57	58	51	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
57	56	55	53	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
44	43	42	30	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
35	36	37	32	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
36	35	34	33	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
64	65	66	54	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
43	44	45	31	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
22	23	15	2	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
20	19	15	2	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
57	58	51	50	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
35	34	33	29	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
43	42	30	29	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
64	63	52	50	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
56	55	53	54	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
57	58	51	53	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
44	45	31	30	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
44	45	31	32	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
65	66	54	52	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
43	42	30	31	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
65	66	54	53	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
64	63	52	54	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
35	34	33	32	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
56	55	53	51	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
36	37	32	33	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
36	37	32	31	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
19	15	2	3	3	0.000	0.000	0.000	-0.000	-0.000	0.000
23	15	2	1	3	0.000	0.000	0.000	-0.000	-0.000	0.000
23	15	2	3	3	0.000	0.000	0.000	-0.000	-0.000	0.000
19	15	2	1	3	0.000	0.000	0.000	-0.000	-0.000	0.000
19	15	2	10	3	0.000	0.000	0.000	-0.000	-0.000	0.000
23	15	2	10	3	0.000	0.000	0.000	-0.000	-0.000	0.000
42	30	29	3	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
58	51	50	1	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
58	51	50	52	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
34	33	29	30	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
42	30	29	33	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
63	52	50	1	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
63	52	50	51	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
34	33	29	3	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
66	54	52	50	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
45	31	30	29	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
55	53	51	50	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
37	32	33	29	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
66	54	52	63	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
58	51	53	55	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
66	54	53	55	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
37	32	33	34	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
45	31	30	42	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
45	31	32	37	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
55	53	54	52	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
45	31	32	33	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
66	54	53	51	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
37	32	31	30	3	9.079	0.000	-9.079	-0.000	-0.000	0.000

34	33	32	31	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
63	52	54	53	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
42	30	31	32	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
58	51	53	54	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
15	2	1	5	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
15	2	3	4	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
3	4	5	1	3	0.628	1.883	0.000	-2.510	-0.000	0.000
30	29	3	4	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
52	50	1	5	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
51	50	1	5	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
33	29	3	4	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
33	29	30	31	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
30	29	3	2	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
51	50	1	2	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
52	50	1	2	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
33	29	3	2	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
54	52	50	1	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
31	30	29	3	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
32	33	29	3	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
53	51	50	1	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
53	51	50	52	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
54	52	50	51	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
32	33	29	30	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
54	53	51	50	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
31	32	33	29	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
32	31	30	29	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
53	54	52	50	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
33	32	31	30	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
52	54	53	51	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
10	2	3	4	3	0.000	0.000	0.000	-0.000	-0.000	0.000
10	2	1	5	3	0.000	0.000	0.000	-0.000	-0.000	0.000
11	6	5	4	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
14	9	4	5	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
14	9	4	3	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
11	6	5	1	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
13	8	9	4	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
12	7	6	5	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
11	6	7	8	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
27	22	23	15	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
26	21	20	19	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
27	22	21	20	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
60	57	56	55	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
47	43	44	45	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
26	21	22	23	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
61	58	57	56	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
68	65	64	63	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
69	64	65	66	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
24	19	15	23	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
48	44	43	42	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
39	35	36	37	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
41	34	35	36	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
40	37	36	35	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
46	42	43	44	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
25	20	19	15	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
28	23	15	19	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
62	55	56	57	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
12	7	8	9	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
13	8	7	6	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
59	56	57	58	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
70	63	64	65	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
28	23	22	21	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
38	36	35	34	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
24	19	20	21	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
67	66	65	64	3	30.334	0.000	-30.334	-0.000	-0.000	0.000

49	45	44	43	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
14	9	8	7	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
25	20	21	22	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
59	56	55	53	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
39	35	34	33	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
48	44	45	31	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
68	65	66	54	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
60	57	58	51	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
47	43	42	30	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
69	64	63	52	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
38	36	37	32	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
28	23	15	2	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
24	19	15	2	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
68	65	66	67	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
41	34	35	39	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
61	58	57	60	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
26	21	20	25	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
69	64	65	68	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
28	23	22	27	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
25	20	19	24	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
62	55	56	59	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
47	43	42	46	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
39	35	36	38	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
12	7	6	11	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
48	44	43	47	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
27	22	21	26	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
60	57	56	59	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
13	8	7	12	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
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61	58	51	50	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
70	63	52	50	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
46	42	30	29	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
41	34	33	29	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
49	45	31	30	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
67	66	54	52	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
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67	66	54	53	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
61	58	51	53	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
49	45	31	32	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
46	42	30	31	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
40	37	32	33	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
41	34	33	32	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
62	55	53	54	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
40	37	32	31	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
70	63	52	54	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
18	10	2	15	3	0.967	2.900	0.000	-3.866	-0.000	0.000
16	10	2	15	3	0.967	2.900	0.000	-3.866	-0.000	0.000
17	10	2	15	3	0.967	2.900	0.000	-3.866	-0.000	0.000
16	10	2	1	3	0.967	2.900	0.000	-3.866	-0.000	0.000
18	10	2	3	3	0.967	2.900	0.000	-3.866	-0.000	0.000
18	10	2	1	3	0.967	2.900	0.000	-3.866	-0.000	0.000
17	10	2	1	3	0.967	2.900	0.000	-3.866	-0.000	0.000
17	10	2	3	3	0.967	2.900	0.000	-3.866	-0.000	0.000
16	10	2	3	3	0.967	2.900	0.000	-3.866	-0.000	0.000

[ pairs ]

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1	9	1
4	7	1



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68 69 1
69 70 1
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#ifdef POSRES
#include "posre.itp"
#endif
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### Atom types (OPLS-AA Force Field)

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; This force field uses a format that requires Gromacs 3.1.4 or later.
;
; References for the OPLS-AA force field:
;
; W. L. Jorgensen, D. S. Maxwell, and J. Tirado-Rives,
; J. Am. Chem. Soc. 118, 11225-11236 (1996).
```

; W. L. Jorgensen and N. A. McDonald, *Theochem* 424, 145-155 (1998).  
 ; W. L. Jorgensen and N. A. McDonald, *J. Phys. Chem. B* 102, 8049-8059 (1998).  
 ; R. C. Rizzo and W. L. Jorgensen, *J. Am. Chem. Soc.* 121, 4827-4836 (1999).  
 ; M. L. Price, D. Ostrovsky, and W. L. Jorgensen, *J. Comp. Chem.* (2001).  
 ; E. K. Watkins and W. L. Jorgensen, *J. Phys. Chem. A* 105, 4118-4125 (2001).  
 ; G. A. Kaminski, R.A. Friesner, J.Tirado-Rives and W.L. Jorgensen, *J. Phys. Chem. B* 105, 6474 (2001).  
 ;

[ defaults ]

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[ atomtypes ]

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opls_842 H842  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_805 C805 12.0110  0.000  A  3.50000E-01  2.76144E-01
opls_833 N833 14.0070  0.000  A  3.25000E-01  7.11280E-01
opls_843 H843  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_846 H846  1.0080  0.000  A  2.42000E-01  1.25520E-01
opls_813 H813  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_844 H844  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_802 C802 12.0110  0.000  A  3.50000E-01  2.76144E-01
opls_815 H815  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_801 C801 12.0110  0.000  A  3.50000E-01  2.76144E-01
opls_822 H822  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_803 C803 12.0110  0.000  A  3.50000E-01  2.76144E-01
opls_834 N834 14.0070  0.000  A  3.25000E-01  7.11280E-01
opls_824 C824 12.0110  0.000  A  3.55000E-01  3.17984E-01
opls_814 H814  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_821 H821  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_823 C823 12.0110  0.000  A  3.55000E-01  2.92880E-01
opls_811 H811  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_838 C838 12.0110  0.000  A  3.55000E-01  3.17984E-01
opls_841 C841 12.0110  0.000  A  3.50000E-01  2.76144E-01
opls_810 H810  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_816 H816  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_831 C831 12.0110  0.000  A  3.55000E-01  3.17984E-01
opls_837 H837  1.0080  0.000  A  2.42000E-01  1.25520E-01
opls_806 C806 12.0110  0.000  A  3.50000E-01  2.76144E-01
opls_836 C836 12.0110  0.000  A  3.55000E-01  3.17984E-01
opls_827 H827  1.0080  0.000  A  2.42000E-01  1.25520E-01
opls_820 C820 12.0110  0.000  A  3.50000E-01  2.76144E-01
opls_835 C835 12.0110  0.000  A  3.55000E-01  2.92880E-01
opls_819 H819  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_804 C804 12.0110  0.000  A  3.50000E-01  2.76144E-01
opls_808 H808  1.0080  0.000  A  0.00000E+00  0.00000E+00
opls_829 C829 12.0110  0.000  A  3.55000E-01  3.17984E-01
opls_845 C845 12.0110  0.000  A  3.55000E-01  3.17984E-01
opls_825 H825  1.0080  0.000  A  2.42000E-01  1.25520E-01
opls_807 H807  1.0080  0.000  A  0.00000E+00  0.00000E+00
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opls_839 H839  1.0080  0.000  A  2.42000E-01  1.25520E-01
opls_812 H812  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_832 H832  1.0080  0.000  A  2.42000E-01  1.25520E-01
opls_809 H809  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_828 C828 12.0110  0.000  A  3.55000E-01  2.92880E-01
opls_817 H817  1.0080  0.000  A  2.50000E-01  1.25520E-01
opls_848 H848  1.0080  0.000  A  2.42000E-01  1.25520E-01
opls_840 C840 12.0110  0.000  A  3.55000E-01  2.92880E-01
opls_830 H830  1.0080  0.000  A  2.42000E-01  1.25520E-01
opls_800 N800 14.0070  0.000  A  3.25000E-01  7.11280E-01
opls_867 H867  1.0080  0.000  A  2.42000E-01  1.25520E-01
opls_814 C814 12.0110  0.000  A  3.50000E-01  2.76144E-01
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opls_820	C820	12.0110	0.000	A	3.50000E-01	3.34720E-01
opls_809	O809	15.9990	0.000	A	2.90000E-01	5.85760E-01
opls_816	C816	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_817	C817	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_858	H858	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_870	C870	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_843	H843	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_848	H848	1.0080	0.000	A	2.42000E-01	1.25520E-01
opls_836	H836	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_835	H835	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_851	H851	1.0080	0.000	A	2.42000E-01	1.25520E-01
opls_834	H834	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_812	O812	15.9990	0.000	A	2.90000E-01	5.85760E-01
opls_860	H860	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_806	O806	15.9990	0.000	A	2.90000E-01	5.85760E-01
opls_811	C811	12.0110	0.000	A	3.50000E-01	2.76144E-01
opls_866	H866	1.0080	0.000	A	2.42000E-01	1.25520E-01
opls_861	H861	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_823	C823	12.0110	0.000	A	3.50000E-01	2.76144E-01
opls_825	O825	15.9990	0.000	A	2.90000E-01	5.85760E-01
opls_857	H857	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_807	C807	12.0110	0.000	A	3.50000E-01	2.76144E-01
opls_875	H875	1.0080	0.000	A	2.42000E-01	1.25520E-01
opls_850	C850	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_822	O822	15.9990	0.000	A	2.90000E-01	5.85760E-01
opls_838	H838	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_818	C818	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_805	C805	12.0110	0.000	A	3.50000E-01	3.34720E-01
opls_827	C827	12.0110	0.000	A	3.50000E-01	2.76144E-01
opls_821	C821	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_844	H844	1.0080	0.000	A	2.42000E-01	1.25520E-01
opls_801	C801	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_847	H847	1.0080	0.000	A	2.42000E-01	1.25520E-01
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opls_832	H832	1.0080	0.000	A	2.50000E-01	1.25520E-01
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opls_829	C829	12.0110	0.000	A	3.50000E-01	2.76144E-01
opls_862	H862	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_833	H833	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_802	C802	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_856	H856	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_813	C813	12.0110	0.000	A	3.50000E-01	2.76144E-01
opls_846	C846	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_849	C849	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_841	H841	1.0080	0.000	A	2.50000E-01	1.25520E-01
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opls_810	C810	12.0110	0.000	A	3.50000E-01	2.76144E-01
opls_855	H855	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_839	H839	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_828	O828	15.9990	0.000	A	2.90000E-01	5.85760E-01
opls_803	C803	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_808	C808	12.0110	0.000	A	3.50000E-01	2.76144E-01
opls_840	H840	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_831	O831	15.9990	0.000	A	2.90000E-01	5.85760E-01

opls_873	H873	1.0080	0.000	A	2.42000E-01	1.25520E-01
opls_854	H854	1.0080	0.000	A	2.50000E-01	1.25520E-01
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opls_830	C830	12.0110	0.000	A	3.50000E-01	2.76144E-01
opls_863	H863	1.0080	0.000	A	2.50000E-01	1.25520E-01
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opls_853	H853	1.0080	0.000	A	2.50000E-01	1.25520E-01
opls_800	C800	12.0110	0.000	A	3.50000E-01	3.34720E-01
opls_871	C871	12.0110	0.000	A	3.55000E-01	2.92880E-01
opls_859	H859	1.0080	0.000	A	2.50000E-01	1.25520E-01
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opls_153	HC 1	1.00800	0.103	A	2.50000e-01	1.25520e-01
opls_401	Cl- 17	35.45300	-1.000	A	4.41724e-01	4.92833e-01
opls_753	NZ 7	14.00670	-0.560	A	3.20000e-01	7.11280e-01
opls_754	CZ 6	12.01100	0.460	A	3.30000e-01	2.76144e-01
opls_755	CT 6	12.01100	-0.080	A	3.30000e-01	2.76144e-01
opls_756	CT 6	12.01100	-0.020	A	3.30000e-01	2.76144e-01
opls_757	CT 6	12.01100	0.040	A	3.30000e-01	2.76144e-01
opls_758	CT 6	12.01100	0.100	A	3.30000e-01	2.76144e-01
opls_759	HC 1	1.00800	0.060	A	2.50000e-01	6.27600e-02
ML	ML 0	0.000000	0.000	A	0.00000e+00	0.00000e+00

### Gro-coordinates file (Molecular rotor, Phe-Orth rotamer)

LIGPARGEN GENERATED GRO FILE

70

1GMR	H00	1	0.100	0.100	0.000
1GMR	C01	2	-0.008	0.100	0.000
1GMR	C02	3	-0.077	0.100	0.122
1GMR	C03	4	-0.077	0.095	-0.120
1GMR	H04	5	-0.022	0.100	0.215
1GMR	C05	6	-0.216	0.095	0.124
1GMR	H06	7	-0.023	0.090	-0.214
1GMR	C07	8	-0.216	0.094	-0.118
1GMR	H08	9	-0.269	0.089	0.218
1GMR	C09	10	-0.285	0.097	0.003
1GMR	C0A	11	-0.310	0.067	-0.228
1GMR	C0B	12	-0.429	0.076	-0.021
1GMR	C0C	13	-0.290	0.099	-0.358
1GMR	C0D	14	-0.431	-0.003	-0.160
1GMR	C0E	15	-0.529	0.118	0.060
1GMR	C0F	16	-0.197	0.205	-0.407
1GMR	C0G	17	-0.351	0.042	-0.482
1GMR	C0H	18	-0.393	-0.151	-0.134
1GMR	C0I	19	-0.562	0.017	-0.239
1GMR	C0J	20	-0.518	0.229	0.159
1GMR	C0K	21	-0.669	0.069	0.072
1GMR	C0M	22	-0.128	0.306	-0.340
1GMR	C0N	23	-0.199	0.206	-0.548
1GMR	C0O	24	-0.440	-0.064	-0.503
1GMR	C0P	25	-0.292	0.103	-0.594
1GMR	C0Q	26	-0.435	-0.217	-0.019
1GMR	C0R	27	-0.312	-0.221	-0.223
1GMR	H0S	28	-0.610	-0.078	-0.265
1GMR	H0T	29	-0.634	0.075	-0.182
1GMR	H0U	30	-0.545	0.071	-0.331
1GMR	C0V	31	-0.420	0.326	0.179
1GMR	C0W	32	-0.640	0.241	0.228
1GMR	C0X	33	-0.738	-0.036	0.012
1GMR	C0Y	34	-0.732	0.140	0.177
1GMR	H0Z	35	-0.130	0.313	-0.233
1GMR	C10	36	-0.056	0.400	-0.413

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1GMR C11 37 -0.127 0.300 -0.621
1GMR H12 38 -0.484 -0.117 -0.421
1GMR C13 39 -0.472 -0.102 -0.633
1GMR C14 40 -0.322 0.064 -0.723
1GMR H15 41 -0.491 -0.164 0.057
1GMR C16 42 -0.405 -0.351 0.002
1GMR H17 43 -0.270 -0.172 -0.310
1GMR C18 44 -0.282 -0.356 -0.203
1GMR H19 45 -0.328 0.324 0.124
1GMR C1A 46 -0.441 0.426 0.273
1GMR C1B 47 -0.661 0.341 0.322
1GMR H1C 48 -0.694 -0.096 -0.065
1GMR C1D 49 -0.868 -0.065 0.052
1GMR C1E 50 -0.862 0.110 0.217
1GMR H1F 51 -0.003 0.478 -0.361
1GMR C1G 52 -0.052 0.395 -0.553
1GMR H1H 53 -0.131 0.300 -0.729
1GMR H1I 54 -0.541 -0.184 -0.648
1GMR C1J 55 -0.416 -0.037 -0.743
1GMR H1K 56 -0.274 0.111 -0.808
1GMR H1M 57 -0.440 -0.400 0.093
1GMR C1N 58 -0.333 -0.423 -0.092
1GMR H1O 59 -0.218 -0.407 -0.274
1GMR H1P 60 -0.364 0.501 0.288
1GMR C1Q 61 -0.559 0.432 0.347
1GMR H1R 62 -0.756 0.349 0.373
1GMR H1S 63 -0.921 -0.147 0.004
1GMR C1T 64 -0.931 0.009 0.151
1GMR H1U 65 -0.907 0.165 0.299
1GMR H1V 66 0.010 0.464 -0.607
1GMR H1W 67 -0.446 -0.066 -0.843
1GMR H1X 68 -0.317 -0.529 -0.080
1GMR H1Y 69 -0.570 0.507 0.425
1GMR H1Z 70 -1.034 -0.012 0.178

```

### Topology file (Molecular rotor, Phe-Orth rotamer)

```

;
; GENERATED BY LigParGen Server
; Jorgensen Lab @ Yale University
;
[ atomtypes ]
opls_863 C863 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_854 C854 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_825 C825 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_858 H858 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_839 C839 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_859 H859 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_844 H844 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_845 C845 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_809 C809 12.0110 0.000 A 3.55000E-01 3.17984E-01
opls_811 C811 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_810 C810 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_817 C817 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_855 H855 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_867 H867 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_818 C818 12.0110 0.000 A 3.50000E-01 2.76144E-01
opls_856 H856 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_828 H828 1.0080 0.000 A 2.50000E-01 1.25520E-01
opls_835 C835 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_852 H852 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_824 C824 12.0110 0.000 A 3.55000E-01 2.92880E-01

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opls_866 H866 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_827 H827 1.0080 0.000 A 2.50000E-01 1.25520E-01
opls_841 C841 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_862 H862 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_860 C860 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_846 C846 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_804 H804 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_829 H829 1.0080 0.000 A 2.50000E-01 1.25520E-01
opls_821 C821 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_814 C814 12.0110 0.000 A 3.55000E-01 3.17984E-01
opls_816 C816 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_840 H840 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_801 C801 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_847 H847 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_819 C819 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_869 H869 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_805 C805 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_807 C807 12.0110 0.000 A 3.55000E-01 3.17984E-01
opls_868 H868 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_837 H837 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_848 C848 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_815 C815 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_832 C832 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_864 H864 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_813 C813 12.0110 0.000 A 3.50000E-01 2.76144E-01
opls_806 H806 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_802 C802 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_812 C812 12.0110 0.000 A 3.55000E-01 3.17984E-01
opls_849 C849 12.0110 0.000 A 3.55000E-01 2.92880E-01
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opls_833 C833 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_850 H850 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_823 C823 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_826 C826 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_830 C830 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_861 H861 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_800 H800 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_803 C803 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_865 H865 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_820 C820 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_857 C857 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_822 C822 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_838 C838 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_808 H808 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_836 C836 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_842 H842 1.0080 0.000 A 2.42000E-01 1.25520E-01
opls_843 C843 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_831 C831 12.0110 0.000 A 3.55000E-01 2.92880E-01
opls_851 C851 12.0110 0.000 A 3.55000E-01 2.92880E-01

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[ moleculetype ]

; Name nrexcl

GMR 3

[ atoms ]

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; nr type resnr residue atom cgnr charge mass
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2 opls_801 1 GMR C01 1 -0.1333 12.0110
3 opls_802 1 GMR C02 1 -0.1333 12.0110
4 opls_803 1 GMR C03 1 -0.1069 12.0110
5 opls_804 1 GMR H04 1 0.1427 1.0080
6 opls_805 1 GMR C05 1 -0.105 12.0110
7 opls_806 1 GMR H06 1 0.1565 1.0080
8 opls_807 1 GMR C07 1 -0.0532 12.0110
9 opls_808 1 GMR H08 1 0.1558 1.0080

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10	opls_809	1	GMR	C09	1	-0.0542	12.0110
11	opls_810	1	GMR	COA	1	-0.0167	12.0110
12	opls_811	1	GMR	COB	1	-0.0172	12.0110
13	opls_812	1	GMR	COC	1	-0.0218	12.0110
14	opls_813	1	GMR	COD	1	0.0863	12.0110
15	opls_814	1	GMR	COE	1	-0.02	12.0110
16	opls_815	1	GMR	COF	1	-0.0496	12.0110
17	opls_816	1	GMR	COG	1	-0.0472	12.0110
18	opls_817	1	GMR	COH	1	-0.0782	12.0110
19	opls_818	1	GMR	COI	1	-0.2413	12.0110
20	opls_819	1	GMR	COJ	1	-0.0488	12.0110
21	opls_820	1	GMR	COK	1	-0.0456	12.0110
22	opls_821	1	GMR	COM	1	-0.1112	12.0110
23	opls_822	1	GMR	CON	1	-0.0488	12.0110
24	opls_823	1	GMR	COO	1	-0.1176	12.0110
25	opls_824	1	GMR	COP	1	-0.0434	12.0110
26	opls_825	1	GMR	COQ	1	-0.1261	12.0110
27	opls_826	1	GMR	COR	1	-0.1269	12.0110
28	opls_827	1	GMR	H0S	1	0.1052	1.0080
29	opls_828	1	GMR	H0T	1	0.1052	1.0080
30	opls_829	1	GMR	H0U	1	0.1052	1.0080
31	opls_830	1	GMR	COV	1	-0.11	12.0110
32	opls_831	1	GMR	COW	1	-0.0486	12.0110
33	opls_832	1	GMR	COX	2	-0.1171	12.0110
34	opls_833	1	GMR	COY	2	-0.0438	12.0110
35	opls_834	1	GMR	H0Z	2	0.1508	1.0080
36	opls_835	1	GMR	C10	2	-0.1388	12.0110
37	opls_836	1	GMR	C11	2	-0.1094	12.0110
38	opls_837	1	GMR	H12	2	0.151	1.0080
39	opls_838	1	GMR	C13	2	-0.1398	12.0110
40	opls_839	1	GMR	C14	2	-0.111	12.0110
41	opls_840	1	GMR	H15	2	0.148	1.0080
42	opls_841	1	GMR	C16	2	-0.1391	12.0110
43	opls_842	1	GMR	H17	2	0.1493	1.0080
44	opls_843	1	GMR	C18	2	-0.1386	12.0110
45	opls_844	1	GMR	H19	2	0.1506	1.0080
46	opls_845	1	GMR	C1A	2	-0.1387	12.0110
47	opls_846	1	GMR	C1B	2	-0.1096	12.0110
48	opls_847	1	GMR	H1C	2	0.1493	1.0080
49	opls_848	1	GMR	C1D	2	-0.1395	12.0110
50	opls_849	1	GMR	C1E	2	-0.1107	12.0110
51	opls_850	1	GMR	H1F	2	0.1393	1.0080
52	opls_851	1	GMR	C1G	2	-0.1344	12.0110
53	opls_852	1	GMR	H1H	2	0.1425	1.0080
54	opls_853	1	GMR	H1I	2	0.1397	1.0080
55	opls_854	1	GMR	C1J	2	-0.1321	12.0110
56	opls_855	1	GMR	H1K	2	0.1433	1.0080
57	opls_856	1	GMR	H1M	2	0.1399	1.0080
58	opls_857	1	GMR	C1N	2	-0.1332	12.0110
59	opls_858	1	GMR	H1O	2	0.1407	1.0080
60	opls_859	1	GMR	H1P	2	0.1393	1.0080
61	opls_860	1	GMR	C1Q	2	-0.1344	12.0110
62	opls_861	1	GMR	H1R	2	0.1427	1.0080
63	opls_862	1	GMR	H1S	2	0.1395	1.0080
64	opls_863	1	GMR	C1T	2	-0.1325	12.0110
65	opls_864	1	GMR	H1U	2	0.1433	1.0080
66	opls_865	1	GMR	H1V	3	0.1396	1.0080
67	opls_866	1	GMR	H1W	3	0.1404	1.0080
68	opls_867	1	GMR	H1X	3	0.139	1.0080
69	opls_868	1	GMR	H1Y	3	0.1396	1.0080
70	opls_869	1	GMR	H1Z	3	0.1404	1.0080

[ bonds ]

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3	2	1	0.1400 392459.200
4	2	1	0.1400 392459.200
5	3	1	0.1080 307105.600
6	3	1	0.1400 392459.200
7	4	1	0.1080 307105.600
8	4	1	0.1433 357313.600
9	6	1	0.1080 307105.600
10	6	1	0.1433 357313.600
11	8	1	0.1433 357313.600
12	10	1	0.1433 357313.600
13	11	1	0.1433 357313.600
14	11	1	0.1495 265265.600
15	12	1	0.1433 357313.600
16	13	1	0.1433 357313.600
17	13	1	0.1433 357313.600
18	14	1	0.1510 265265.600
19	14	1	0.1529 224262.400
20	15	1	0.1433 357313.600
21	15	1	0.1433 357313.600
22	16	1	0.1400 392459.200
23	16	1	0.1424 392459.200
24	17	1	0.1400 392459.200
25	17	1	0.1424 392459.200
26	18	1	0.1400 392459.200
27	18	1	0.1400 392459.200
28	19	1	0.1090 284512.000
29	19	1	0.1090 284512.000
30	19	1	0.1090 284512.000
31	20	1	0.1400 392459.200
32	20	1	0.1424 392459.200
33	21	1	0.1400 392459.200
34	21	1	0.1424 392459.200
35	22	1	0.1080 307105.600
36	22	1	0.1400 392459.200
37	23	1	0.1400 392459.200
38	24	1	0.1080 307105.600
39	24	1	0.1400 392459.200
40	25	1	0.1400 392459.200
41	26	1	0.1080 307105.600
42	26	1	0.1400 392459.200
43	27	1	0.1080 307105.600
44	27	1	0.1400 392459.200
45	31	1	0.1080 307105.600
46	31	1	0.1400 392459.200
47	32	1	0.1400 392459.200
48	33	1	0.1080 307105.600
49	33	1	0.1400 392459.200
50	34	1	0.1400 392459.200
51	36	1	0.1080 307105.600
52	36	1	0.1400 392459.200
53	37	1	0.1080 307105.600
54	39	1	0.1080 307105.600
55	39	1	0.1400 392459.200
56	40	1	0.1080 307105.600
57	42	1	0.1080 307105.600
58	42	1	0.1400 392459.200
59	44	1	0.1080 307105.600
60	46	1	0.1080 307105.600
61	46	1	0.1400 392459.200
62	47	1	0.1080 307105.600
63	49	1	0.1080 307105.600
64	49	1	0.1400 392459.200
65	50	1	0.1080 307105.600
66	52	1	0.1080 307105.600

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67 55 1 0.1080 307105.600
68 58 1 0.1080 307105.600
69 61 1 0.1080 307105.600
70 64 1 0.1080 307105.600
10 8 1 0.1460 322168.000
14 12 1 0.1495 265265.600
25 23 1 0.1424 392459.200
34 32 1 0.1424 392459.200
52 37 1 0.1400 392459.200
55 40 1 0.1400 392459.200
58 44 1 0.1400 392459.200
61 47 1 0.1400 392459.200
64 50 1 0.1400 392459.200

```

[ angles ]

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; ai aj ak funct c0 c1 c2 c3
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1 2 4 1 120.000 292.880
2 3 5 1 120.000 292.880
2 3 6 1 120.000 527.184
2 4 7 1 120.000 292.880
2 4 8 1 124.000 585.760
3 6 9 1 120.000 292.880
3 6 10 1 124.000 585.760
4 8 11 1 115.690 382.752
6 10 12 1 115.690 382.752
8 11 13 1 119.200 525.092
8 11 14 1 119.200 525.092
10 12 15 1 119.200 525.092
11 13 16 1 115.690 382.752
11 13 17 1 115.690 382.752
11 14 18 1 109.500 334.720
11 14 19 1 115.600 527.184
12 15 20 1 115.690 382.752
12 15 21 1 115.690 382.752
13 16 22 1 124.000 585.760
13 16 23 1 124.000 585.760
13 17 24 1 124.000 585.760
13 17 25 1 124.000 585.760
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14 18 27 1 120.000 585.760
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21 33 49 1 120.000 527.184
21 34 50 1 120.000 527.184
22 36 51 1 120.000 292.880

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22	36	52	1	120.000	527.184
23	37	53	1	120.000	292.880
24	39	54	1	120.000	292.880
24	39	55	1	120.000	527.184
25	40	56	1	120.000	292.880
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26	42	58	1	120.000	527.184
27	44	59	1	120.000	292.880
31	46	60	1	120.000	292.880
31	46	61	1	120.000	527.184
32	47	62	1	120.000	292.880
33	49	63	1	120.000	292.880
33	49	64	1	120.000	527.184
34	50	65	1	120.000	292.880
36	52	66	1	120.000	292.880
39	55	67	1	120.000	292.880
42	58	68	1	120.000	292.880
46	61	69	1	120.000	292.880
49	64	70	1	120.000	292.880
7	4	8	1	118.990	539.820
38	24	39	1	120.000	292.880
21	34	32	1	120.000	527.184
44	58	68	1	120.000	292.880
47	61	69	1	120.000	292.880
6	10	8	1	117.000	711.280
57	42	58	1	120.000	292.880
43	27	44	1	120.000	292.880
12	14	19	1	115.600	527.184
16	23	25	1	120.000	527.184
8	10	12	1	117.000	711.280
27	44	58	1	120.000	527.184
46	61	47	1	120.000	527.184
34	32	47	1	120.000	527.184
4	8	10	1	117.000	711.280
49	64	50	1	120.000	527.184
10	8	11	1	117.000	711.280
40	55	67	1	120.000	292.880
52	37	53	1	120.000	292.880
54	39	55	1	120.000	292.880
63	49	64	1	120.000	292.880
31	20	32	1	120.000	527.184
61	47	62	1	120.000	292.880
20	15	21	1	115.690	382.752
28	19	29	1	107.800	276.144
39	55	40	1	120.000	527.184
55	40	56	1	120.000	292.880
18	14	19	1	114.000	527.184
11	14	12	1	109.500	334.720
9	6	10	1	118.990	539.820
12	14	18	1	109.500	334.720
13	11	14	1	119.200	525.092
35	22	36	1	120.000	292.880
5	3	6	1	120.000	292.880
33	21	34	1	120.000	527.184
28	19	30	1	107.800	276.144
24	17	25	1	120.000	527.184
14	12	15	1	119.200	525.092
29	19	30	1	107.800	276.144
51	36	52	1	120.000	292.880
25	23	37	1	120.000	527.184
58	44	59	1	120.000	292.880
50	64	70	1	120.000	292.880
37	52	66	1	120.000	292.880
32	34	50	1	120.000	527.184

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17 25 23 1 120.000 527.184
42 58 44 1 120.000 527.184
45 31 46 1 120.000 292.880
32 47 61 1 120.000 527.184
23 25 40 1 120.000 527.184
60 46 61 1 120.000 292.880
20 32 34 1 120.000 527.184
3 2 4 1 120.000 527.184
25 40 55 1 120.000 527.184
64 50 65 1 120.000 292.880
10 12 14 1 119.200 525.092
34 50 64 1 120.000 527.184
16 13 17 1 115.690 382.752
23 37 52 1 120.000 527.184
22 16 23 1 120.000 527.184
26 18 27 1 120.000 527.184
48 33 49 1 120.000 292.880
41 26 42 1 120.000 292.880
36 52 37 1 120.000 527.184

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[ dihedrals ]

; IMPROPER DIHEDRAL ANGLES

; ai	aj	ak	al	funct	c0	c1	c2	c3	c4	c5
8	4	2	7	4	180.000	10.460	2			
10	6	3	9	4	180.000	10.460	2			
15	12	10	14	4	180.000	10.460	2			
64	49	33	63	4	180.000	10.460	2			
61	46	31	60	4	180.000	10.460	2			
58	42	26	57	4	180.000	10.460	2			
55	39	24	54	4	180.000	10.460	2			
52	36	22	51	4	180.000	10.460	2			
6	3	2	5	4	180.000	10.460	2			
44	27	18	43	4	180.000	10.460	2			
42	26	18	41	4	180.000	10.460	2			
49	33	21	48	4	180.000	10.460	2			
36	22	16	35	4	180.000	10.460	2			
46	31	20	45	4	180.000	10.460	2			
39	24	17	38	4	180.000	10.460	2			
27	18	14	26	4	180.000	10.460	2			
4	2	1	3	4	180.000	10.460	2			
37	23	16	25	4	180.000	10.460	2			
50	34	21	32	4	180.000	10.460	2			
47	32	20	34	4	180.000	10.460	2			
40	25	17	23	4	180.000	10.460	2			
11	8	4	10	4	180.000	10.460	2			
12	10	6	8	4	180.000	10.460	2			
17	13	11	16	4	180.000	10.460	2			
21	15	12	20	4	180.000	10.460	2			
34	21	15	33	4	180.000	10.460	2			
32	20	15	31	4	180.000	10.460	2			
25	17	13	24	4	180.000	10.460	2			
23	16	13	22	4	180.000	10.460	2			
14	11	8	13	4	180.000	10.460	2			
68	58	42	44	4	180.000	10.460	2			
69	61	46	47	4	180.000	10.460	2			
59	44	27	58	4	180.000	10.460	2			
70	64	49	50	4	180.000	10.460	2			
67	55	39	40	4	180.000	10.460	2			
66	52	36	37	4	180.000	10.460	2			
56	40	25	55	4	180.000	10.460	2			
53	37	23	52	4	180.000	10.460	2			
65	50	34	64	4	180.000	10.460	2			
62	47	32	61	4	180.000	10.460	2			

[ dihedrals ]

; PROPER DIHEDRAL ANGLES

; ai	aj	ak	al	funct	c0	c1	c2	c3	c4	c5
8	10	6	3	3	16.027	-4.391	-14.029	2.393	-0.000	0.000
10	8	4	2	3	16.027	-4.391	-14.029	2.393	-0.000	0.000
10	8	4	7	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
8	4	2	3	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
10	6	3	2	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
10	6	3	5	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
8	4	2	1	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
13	11	8	10	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
15	12	10	8	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
15	12	10	6	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
13	11	8	4	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
15	12	14	11	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
13	11	14	12	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
6	10	8	4	3	0.628	1.883	0.000	-2.510	-0.000	0.000
58	42	26	18	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
58	44	27	18	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
50	64	49	33	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
44	58	42	26	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
42	58	44	27	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
42	26	18	27	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
47	61	46	31	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
37	52	36	22	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
40	55	39	24	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
44	27	18	26	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
6	3	2	4	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
61	46	31	20	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
36	52	37	23	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
46	61	47	32	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
39	55	40	25	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
52	36	22	16	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
55	39	24	17	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
64	49	33	21	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
49	64	50	34	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
42	26	18	14	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
44	27	18	14	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
55	39	24	38	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
64	49	33	48	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
52	36	22	35	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
61	46	31	45	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
58	42	26	41	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
58	44	27	43	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
6	3	2	1	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
46	31	20	15	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
36	22	16	13	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
39	24	17	13	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
49	33	21	15	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
36	22	16	23	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
64	50	34	21	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
39	24	17	25	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
64	50	34	32	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
55	40	25	17	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
46	31	20	32	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
52	37	23	16	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
55	40	25	23	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
52	37	23	25	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
49	33	21	34	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
61	47	32	20	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
61	47	32	34	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
27	18	14	11	3	0.000	0.000	0.000	-0.000	-0.000	0.000
26	18	14	12	3	0.000	0.000	0.000	-0.000	-0.000	0.000
26	18	14	11	3	0.000	0.000	0.000	-0.000	-0.000	0.000
27	18	14	12	3	0.000	0.000	0.000	-0.000	-0.000	0.000
26	18	14	19	3	0.000	0.000	0.000	-0.000	-0.000	0.000

27	18	14	19	3	0.000	0.000	0.000	-0.000	-0.000	0.000
24	17	13	11	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
22	16	13	11	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
33	21	15	20	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
33	21	15	12	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
31	20	15	21	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
24	17	13	16	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
22	16	13	17	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
31	20	15	12	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
50	34	21	15	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
47	32	20	15	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
40	25	17	13	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
37	23	16	13	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
50	34	32	47	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
40	25	23	37	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
40	25	17	24	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
50	34	21	33	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
37	23	16	22	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
47	32	20	31	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
50	34	32	20	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
40	25	23	16	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
24	17	25	23	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
47	32	34	21	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
33	21	34	32	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
37	23	25	17	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
18	14	12	10	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
18	14	11	8	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
18	14	12	15	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
18	14	11	13	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
11	8	10	6	3	0.628	1.883	0.000	-2.510	-0.000	0.000
12	10	8	4	3	0.628	1.883	0.000	-2.510	-0.000	0.000
12	10	8	11	3	0.628	1.883	0.000	-2.510	-0.000	0.000
12	10	6	3	3	16.027	-4.391	-14.029	2.393	-0.000	0.000
11	8	4	2	3	16.027	-4.391	-14.029	2.393	-0.000	0.000
12	10	6	9	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
11	8	4	7	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
21	15	12	10	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
17	13	11	8	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
16	13	11	8	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
20	15	12	10	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
16	13	11	14	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
21	15	12	14	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
17	13	11	14	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
20	15	12	14	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
32	20	15	12	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
32	20	15	21	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
34	21	15	20	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
25	17	13	16	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
34	21	15	12	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
23	16	13	11	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
25	17	13	11	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
23	16	13	17	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
25	23	16	13	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
23	25	17	13	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
34	32	20	15	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
32	34	21	15	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
25	23	16	22	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
34	32	20	31	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
21	34	32	20	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
17	25	23	16	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
11	14	12	10	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
12	14	11	8	3	9.079	0.000	-9.079	-0.000	-0.000	0.000
14	11	8	10	3	0.527	-6.397	-1.695	7.565	-0.000	0.000
14	12	10	8	3	0.527	-6.397	-1.695	7.565	-0.000	0.000

14	12	10	6	3	58.576	0.000	-58.576	-0.000	-0.000	0.000
14	11	8	4	3	58.576	0.000	-58.576	-0.000	-0.000	0.000
19	14	12	10	3	0.000	0.000	0.000	-0.000	-0.000	0.000
19	14	12	15	3	0.000	0.000	0.000	-0.000	-0.000	0.000
19	14	11	13	3	0.000	0.000	0.000	-0.000	-0.000	0.000
19	14	11	8	3	0.000	0.000	0.000	-0.000	-0.000	0.000
9	6	10	8	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
63	49	64	50	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
59	44	27	18	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
68	58	42	26	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
70	64	49	33	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
56	40	55	39	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
60	46	61	47	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
41	26	18	27	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
9	6	3	2	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
59	44	58	42	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
5	3	2	4	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
54	39	55	40	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
66	52	36	22	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
65	50	64	49	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
69	61	46	31	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
43	27	18	26	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
51	36	52	37	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
62	47	61	46	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
67	55	39	24	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
57	42	26	18	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
68	58	44	27	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
57	42	58	44	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
7	4	2	3	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
53	37	52	36	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
66	52	37	23	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
54	39	24	17	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
67	55	40	25	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
63	49	33	21	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
69	61	47	32	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
60	46	31	20	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
70	64	50	34	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
51	36	22	16	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
43	27	18	14	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
41	26	18	14	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
9	6	3	5	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
70	64	49	63	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
57	42	26	41	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
59	44	27	43	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
60	46	31	45	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
68	58	44	59	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
67	55	40	56	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
67	55	39	54	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
54	39	24	38	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
5	3	2	1	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
70	64	50	65	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
63	49	33	48	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
51	36	22	35	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
66	52	37	53	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
68	58	42	57	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
66	52	36	51	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
7	4	2	1	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
69	61	46	60	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
69	61	47	62	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
35	22	16	13	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
48	33	21	15	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
38	24	17	13	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
45	31	20	15	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
65	50	34	21	3	30.334	0.000	-30.334	-0.000	-0.000	0.000



56	40	25	17	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
53	37	23	25	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
38	24	17	25	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
45	31	20	32	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
62	47	32	20	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
65	50	34	32	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
53	37	23	16	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
62	47	32	34	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
48	33	21	34	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
56	40	25	23	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
35	22	16	23	3	30.334	0.000	-30.334	-0.000	-0.000	0.000
28	19	14	18	3	0.967	2.900	0.000	-3.866	-0.000	0.000
30	19	14	18	3	0.967	2.900	0.000	-3.866	-0.000	0.000
29	19	14	18	3	0.967	2.900	0.000	-3.866	-0.000	0.000
29	19	14	12	3	0.967	2.900	0.000	-3.866	-0.000	0.000
30	19	14	11	3	0.967	2.900	0.000	-3.866	-0.000	0.000
28	19	14	11	3	0.967	2.900	0.000	-3.866	-0.000	0.000
28	19	14	12	3	0.967	2.900	0.000	-3.866	-0.000	0.000
29	19	14	11	3	0.967	2.900	0.000	-3.866	-0.000	0.000
30	19	14	12	3	0.967	2.900	0.000	-3.866	-0.000	0.000

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```
#ifdef POSRES
#include "posre.itp"
#endif
```