

Supplementary

Optimization of the OPLS-AA Force Field for Long Hydrocarbons by

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This supplementary contains the *ab initio* torsional potentials for n-hexane, cis-3-hexene, and cis-2-hexene.

n-HEXANE torsion C5-C8-C11-C14

dihedral	Relative energy [kJ/mol]
-90	5.9991599668283015
-88	5.4382846708176658
-86	4.9154564866330475
-84	4.4299599735531956
-82	3.9907039143145084
-80	3.5978611621540040
-78	3.2493252772837877
-76	2.9454487242037430
-74	2.6924685594858602
-72	2.4763692679116502
-70	2.3072238862514496
-68	2.1842585131525993
-66	2.1005592140136287
-64	2.0684642696287483
-62	2.0954405484953895
-60	2.1861192237120122
-58	2.3347879732027650
-56	2.5568047049455345
-54	2.8493083523353562
-52	3.2177897616056725
-50	3.6595108004985377
-48	4.1805213850457221
-46	4.7753010713495314
-44	5.4390951670939103
-42	6.1695172328036278
-40	6.9638311136513948
-38	7.8146846066229045
-36	8.7145440600579605
-34	9.6525528429774567
-32	10.6263526355614886
-30	11.6223734056111425
-28	12.6344116455875337
-26	13.6524734371341765
-24	14.6638867487199605
-22	15.661439006332394
-20	16.6306449297117069
-18	17.5604039125610143
-16	18.4499422821681947
-14	19.2533267323160544
-12	19.9958248498151079
-10	20.6572516862070188

-8	21.2167556725908071
-6	21.6667014787672088
-4	21.9970236589433625
-2	22.1988018063129857
0	22.2662540067685768
2	22.1977247931063175
4	21.9965970416087657
6	21.6680261376313865
8	21.2167210162151605
10	20.6575807158369571
12	19.9974901148816571
14	19.2550191476475447
16	18.4497240278869867
18	17.5597305638948455
20	16.6291635815287009
22	15.6601879184599966
24	14.6663141680182889
26	13.6514879500027746
28	12.6340421988861635
30	11.6224943335400894
32	10.6248722021700814
34	9.6522809301968664
36	8.7136564349057153
38	7.8156212255125865
40	6.9647408303571865
42	6.1694607083918527
44	5.4376755678094923
46	4.7751592923887074
48	4.1809534900821745
50	3.6604948071762919
52	3.2165907206945121
54	2.8500621531857178
56	2.5591596259037033
58	2.3527258062968031
60	2.1875826182076707
62	2.0937077195849270
64	2.0700464968103915
66	2.1008879190776497
68	2.1840835536131635
70	2.3070087215164676
72	2.4763896132353693
74	2.6919824815122411
76	2.9455995121970773
78	3.2490007421001792
80	3.5980503179598600
82	3.9941250896081328
84	4.4311096214223653
86	4.9145311409374699
88	5.4404005178948864
90	5.9989143981365487
92	6.5849235682981089
94	7.1900247448356822
96	7.8019692478701472
98	8.4078441566089168
100	9.0039103874005377
102	9.5747761602979153

104	10.1125125563703477
106	10.6101065491093323
108	11.0558497293386608
110	11.4461674897465855
112	11.7717265874380246
114	12.0291313180932775
116	12.2126714756013826
118	12.3250143268378451
120	12.3618128662928939
122	12.3213886717567220
124	12.2084518872434273
126	12.0203076055040583
128	11.7621381666976959
130	11.4392882529646158
132	11.0547933394555002
134	10.6152970039984211
136	10.1250354346120730
138	9.5914842232596129
140	9.0217576534487307
142	8.4233764961827546
144	7.8025257362751290
146	7.1667648445582017
148	6.5237202740972862
150	5.8800162809202448
152	5.2409978859359398
154	4.6163164884783328
156	4.0106342849321663
158	3.4301297527272254
160	2.8808020178694278
162	2.3660169510403648
164	1.8939092289656401
166	1.4658856081077829
168	1.0876619605114684
170	0.7622344377450645
172	0.4906349325319752
174	0.2777549722231925
176	0.1253776617813855
178	0.0317422964144498
180	0.0000000000000000
182	0.0319638929795474
184	0.1243540855357423
186	0.2776032277615741
188	0.4914134828140959
190	0.7608710915083066
192	1.0875733356224373
194	1.4663116690935567
196	1.8941225508460775
198	2.3657786683179438
200	2.8802966480143368
202	3.4296133042080328
204	4.0104664146201685
206	4.6165835735155270
208	5.2404950649943203
210	5.8784823236055672
212	6.5232230453984812
214	7.1661441124742851

216	7.8018023271579295
218	8.4225499883759767
220	9.0220401317346841
222	9.5908807852538303
224	10.1246463287388906
226	10.6151808343129233
228	11.0557170301908627
230	11.4413836690364406
232	11.7619863561121747
234	12.0210842986125499
236	12.2069832691922784
238	12.3219057106180117
240	12.3622549746651202
242	12.3255527840228751
244	12.2117400571005419
246	12.0283203801373020
248	11.7719678957946599
250	11.4453803306678310
252	11.0561034807469696
254	10.6104826985392720
256	10.1141626335447654
258	9.5747859526891261
260	9.0034997514449060
262	8.4080452744383365
264	7.8027043415931985
266	7.1894768916536123
268	6.5844638962298632

CIS-3-HEXENE

torsion C5-C8=C10-C12

dihedral Relative energy [kJ/mol]

-88	138.8696708501083776
-86	132.9265517032472417
-84	127.0755713694961742
-82	121.3217440731823444
-80	115.6625391189008951
-78	110.1054139159386978
-76	104.6512541139964014
-74	99.3135456056334078
-72	94.0864945350913331
-70	88.9759613954229280
-68	83.9913259764434770
-66	79.1386741471942514
-64	74.4164158123312518
-62	69.8332949931500480
-60	65.3922178068896756
-58	61.0939228800125420
-56	56.9470554657746106
-54	52.9486835125135258
-52	49.1006604022113606
-50	45.4035276250215247
-48	41.8641888723941520
-46	38.4787404485978186
-44	35.2465835297480226
-42	32.1636756988009438

-40	29.2383331460878253
-38	26.4628684573108330
-36	23.8370954362908378
-34	21.3569554293062538
-32	19.0250233793631196
-30	16.8371324953623116
-28	14.7843290625605732
-26	12.8768097991123796
-24	11.1043524676933885
-22	9.4662862529512495
-20	7.9646190571365878
-18	6.5917739175492898
-16	5.3446827986044809
-14	4.2394922144012526
-12	3.2542275751475245
-10	2.3950888360850513
-8	1.6606338226702064
-6	1.0535754117881879
-4	0.5729611305287108
-2	0.2144161238102242
0	0.0000000000000000
2	0.2169851588550955
4	0.5744696349138394
6	1.0591332268668339
8	1.6623312989249825
10	2.3914549882756546
12	3.2538216749671847
14	4.2386236721649766
16	5.3513955823145807
18	6.5896979722892866
20	7.9645108962431550
22	9.4658509900327772
24	11.1049456647597253
26	12.8746930895140395
28	14.7855282466625795
30	16.8364856205880642
32	19.0224190126173198
34	21.3581209565745667
36	23.8388846382731572
38	26.4629445287864655
40	29.2456601248122752
42	32.1642074292758480
44	35.2446513683535159
46	38.4915880092885345
48	41.8614983262959868
50	45.3998212813166901
52	49.0961660484317690
54	52.9451007843017578
56	56.9430516528664157
58	61.0976281722541898
60	65.3924997658468783
62	69.8345177049050108
64	74.4125332217663527
66	79.1374072104226798
68	83.9953360207146034
70	88.9789946607779711

72	94.0767527098068967
74	99.3134557029698044
76	104.6515650963410735
78	110.1079450844554231
80	115.6630859838332981
82	121.3216070514172316
84	127.0809748799074441
86	132.9271745125297457
88	138.8703704604413360

CIS-2-HEXENE
torsion C5=C7-C9-C12

dihedral	Relative energy [kJ/mol]
-90	0.3644080035155639
-88	0.4538847481599078
-86	0.5673571289516985
-84	0.6897001350298524
-82	0.8504762942902744
-80	1.0380542562343180
-78	1.2753777536563575
-76	1.5498677302384749
-74	1.8831514193443581
-72	2.2768710221862420
-70	2.7336917776847258
-68	3.2606272106058896
-66	3.8534488020231947
-64	4.5244999642018229
-62	5.2516263776924461
-60	6.0533313712803647
-58	6.9059446267783642
-56	7.7939434930449352
-54	8.7196963179158047
-52	9.6464032795047387
-50	10.5738815516233444
-48	11.4684767535654828
-46	12.3244555878918618
-44	13.1075043138116598
-42	13.8174476951826364
-40	14.4520392604172230
-38	14.9993045285809785
-36	15.4738580104894936
-34	15.8775472262641415
-32	16.2184218371985480
-30	16.8531041881069541
-28	16.8695421678712592
-26	16.7810253989882767
-24	16.6651021355064586
-22	16.5198372323065996
-20	16.3660631179809570
-18	16.2092548360815272
-16	16.0528412312269211
-14	15.9071553166722879
-12	15.7738251821137965
-10	15.6568245158996433

-8	15.5578347598202527
-6	15.4789025338832289
-4	15.4213869293453172
-2	15.3865406854311004
0	15.3749921926064417
2	15.3866211326094344
4	15.4213844250189140
6	15.4788952778326347
8	15.5578915636288002
10	15.6572453423868865
12	15.7751260583754629
14	15.9083190276287496
16	16.0537932493025437
18	16.2071933703264222
20	17.3568218656582758
22	17.2569123649736866
24	17.1219379795948043
26	16.9778551041381434
28	16.7510588472941890
30	16.5141683992696926
32	16.2178642998915166
34	15.8823376068612561
36	15.4732025358825922
38	14.9959623060422018
40	14.4513460556045175
42	13.8277072721393779
44	13.1070847334340215
46	12.3230009373510256
48	11.4677009048173204
50	10.5714735337533057
52	9.6461819398682564
54	8.7159575675614178
56	7.7945871707051992
58	6.9045614071656018
60	6.0544261656468734
62	5.2573874326189980
64	4.5240784027846530
66	3.8666138451080769
68	3.2605984265683219
70	2.7326363063184544
72	2.2766646078089252
74	1.8833693921333179
76	1.5497630662284791
78	1.2728795980801806
80	1.0382058779941872
82	0.8472705368185416
84	0.6893653915030882
86	0.5626404401846230
88	0.4536086900625378
90	0.3649183401139453
92	0.2893518415512517
94	0.2220795579487458
96	0.1692852501291782
98	0.1225096095586196
100	0.0802498166449368
102	0.0456134369596839

104	0.0209538011113182
106	0.0095028385985643
108	0.0000000000000000
110	0.0067321291426197
112	0.0219271351816133
114	0.0533579824259505
116	0.0942983182612807
118	0.1507120096357539
120	0.2212366510648280
122	0.3052308050682768
124	0.4045219704275951
126	0.5178893628763035
128	0.6433573368703946
130	0.7819680884713307
132	0.9361937127541751
134	1.1009921682998538
136	1.2782101053744555
138	1.4645795274991542
140	1.6617082052398473
142	1.8628291280474514
144	2.0740120238624513
146	2.2843012652592734
148	2.4987001576228067
150	2.7083505763439462
152	2.9157246970571578
154	3.1139420474646613
156	3.3060694389278069
158	3.4871605697553605
160	3.6519067478366196
162	3.8050902081886306
164	3.9403656212380156
166	4.0615517215337604
168	4.1641594789689407
170	4.2524004558799788
172	4.3211819450370967
174	4.3757776406127959
176	4.4138798523927107
178	4.4370969856390730
180	4.4443721714196727
182	4.4373641558922827
184	4.4138604262843728
186	4.3739202247234061
188	4.3230451305862516
190	4.2516388823278248
192	4.1647122949361801
194	4.0639889778103679
196	3.9416266147745773
198	3.8057263916125521
200	3.6527057148050517
202	3.4852709239348769
204	3.3066772916354239
206	3.1149458191357553
208	2.9161636469652876
210	2.7105736943194643
212	2.4987442370038480
214	2.2890187773155048

216	2.0744829009054229
218	1.8688951026415452
220	1.6619956350186840
222	1.4693994157714769
224	1.2783863218501210
226	1.1032427767058834
228	0.9364138969685882
230	0.7844123154645786
232	0.6438206469174474
234	0.5179003443336114
236	0.4045696917455643
238	0.3062579309334978
240	0.2214666964719072
242	0.1507390915649012
244	0.0944875889690593
246	0.0521617623744532
248	0.0222142330603674
250	0.0043847721535712
252	0.0001339771552011
254	0.0044866704847664
256	0.0217902943259105
258	0.0433952091261744
260	0.0804229587083682
262	0.1236633296357468
264	0.1696563605219126
266	0.2295113224536180
268	0.2895989295793697

CIS-2-HEXENE
torsion C7-C9-C12-C15

dihedral	Relative energy [kJ/mol]
-90	5.6825760897481814
-88	4.8321663094684482
-86	4.0267469220561907
-84	3.2605444105574861
-82	2.5566971888765693
-80	1.9245065491413698
-78	1.3674022624036297
-76	0.8983700525714085
-74	0.5418334254063666
-72	0.2578457590425387
-70	0.0772718256339431
-68	0.0000000000000000
-66	0.0013560472289100
-64	0.1110178937669843
-62	0.3314471412450075
-60	0.6239353618584573
-58	0.9925275852438062
-56	1.4385272228391841
-54	1.9568123593926430
-52	2.5411144641693681
-50	3.2018649289384484
-48	3.9282783713424578
-46	4.7050433515105397

-44	5.5385061646811664
-42	6.4222343211295083
-40	7.3647311050444841
-38	8.3170064256992191
-36	9.3172299228608608
-34	10.3377079028869048
-32	11.3678346290253103
-30	12.3938969731098041
-28	13.3997643877519295
-26	14.3938525948906317
-24	15.3695761488052085
-22	16.3009708287427202
-20	17.1945575108984485
-18	18.0359719446860254
-16	18.8057920414721593
-14	19.5101235427428037
-12	20.1445710536791012
-10	20.6989129219437018
-8	21.1576685605105013
-6	21.5308086503064260
-4	21.8062637419207022
-2	21.9602992216823623
0	22.0044574404601008
2	21.9232915210304782
4	21.7193875560769811
6	21.3949979675235227
8	20.9577791176270694
10	20.4268586037214845
12	19.7998474634950981
14	19.0943462938303128
16	18.3198691590223461
18	17.4901343575911596
20	16.6105124128516763
22	15.6968207136960700
24	14.7584387136157602
26	13.7990767144365236
28	12.8339858168037608
30	11.8776715721469373
32	10.9324680796125904
34	10.0062333452515304
36	9.1129041882231832
38	8.2542902047280222
40	7.4438144661253318
42	6.6836531790904701
44	5.9823930045822635
46	5.3477799516404048
48	4.7842419235967100
50	4.2924270804505795
52	3.8821073939325288
54	3.5527894991682842
56	3.3150783469900489
58	3.1518986851442605
60	3.0808366975979879
62	3.1014439505524933
64	3.2178940438898280
66	3.4020780209684744

68	3.6844472212251276
70	4.0416095957625657
72	4.4773140923352912
74	5.0165695321047679
76	5.6166530981427059
78	6.2218342217383906
80	6.8106716834008694
82	7.4121847907081246
84	8.0320467646233737
86	8.6713780933059752
88	9.3357435729121789
90	10.0225989525206387
92	10.7175537395523861
94	11.4155221127439290
96	12.1072683118982241
98	12.7738613559631631
100	13.4191249147988856
102	14.0118873537285253
104	14.5593011833261698
106	15.0505818121600896
108	15.4696605103090405
110	15.8230629608733580
112	16.0968728899024427
114	16.2815773811889812
116	16.3874543005367741
118	16.3975892983144149
120	16.3227604187559336
122	16.1642155139707029
124	15.9198579877847806
126	15.5974306829739362
128	15.1972165808547288
130	14.7303715675370768
132	14.1964998085750267
134	13.6092201969586313
136	12.9680560560664162
138	12.2923114032018930
140	11.5794284555595368
142	10.8423594685737044
144	10.0892302575521171
146	9.3263463373295963
148	8.5627048868918791
150	7.8110759799601510
152	7.0725533624645323
154	6.3593628586968407
156	5.6711364869261160
158	5.0317545525031164
160	4.4303246267372742
162	3.8803068426204845
164	3.3844694716390222
166	2.9503753127064556
168	2.5876531091053039
170	2.2767712960485369
172	2.0497486711246893
174	1.8856538980035111
176	1.8040376630378887
178	1.7887489250861108

180	1.8560300847748294
182	1.9892772303428501
184	2.1969017750816420
186	2.4790525450371206
188	2.8164474004879594
190	3.2361491974443197
192	3.7064364611869678
194	4.2307238904759288
196	4.7969928683014587
198	5.4213522181380540
200	6.0812172848964110
202	6.7642468063859269
204	7.4706539751496166
206	8.2036157079273835
208	8.9393465783214197
210	9.6816495833918452
212	10.4137961500091478
214	11.1346528056310490
216	11.8305351000744849
218	12.4964537407504395
220	13.1250975728034973
222	13.7027045238064602
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230	15.4038157282629982
232	15.6434730817563832
234	15.7976667893817648
236	15.8684867010451853
238	15.8393969946773723
240	15.7257082622963935
242	15.5157778221182525
244	15.2256101650418714
246	14.8304594656219706
248	14.3626159285195172
250	13.8080453965812922
252	13.1886927408631891
254	12.4927406139904633
256	11.7481498823035508
258	10.9437094570603222
260	10.1082801728043705
262	9.2358886072179303
264	8.3543197767576203
266	7.4522076825378463
268	6.5605715528363362