Electronic supplementary information

Theoretical studies on a carbonaceous molecular bearing: Association thermodynamics and dual-mode rolling dynamics

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Supporting Figures

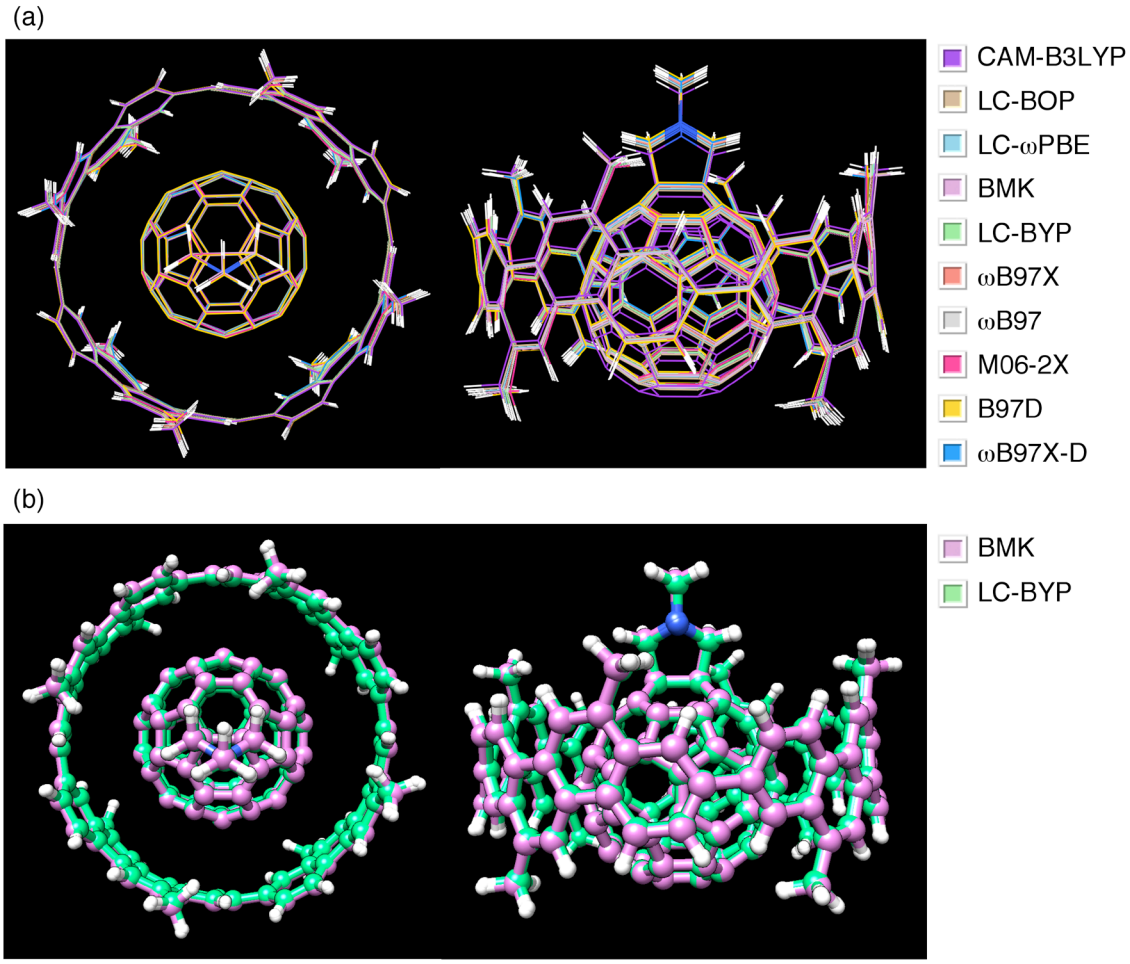

Fig. S1. Geometry-optimized molecular structures of (*P*)-(12,8)-[4]CC⊃**1** from DFT calculations. Carbon atoms are colored separately. (a) All the geometries were overlaid with RMSD of 0.195 Å. (b) Two representative geometries were overlaid with RMSD of 0.090 Å.

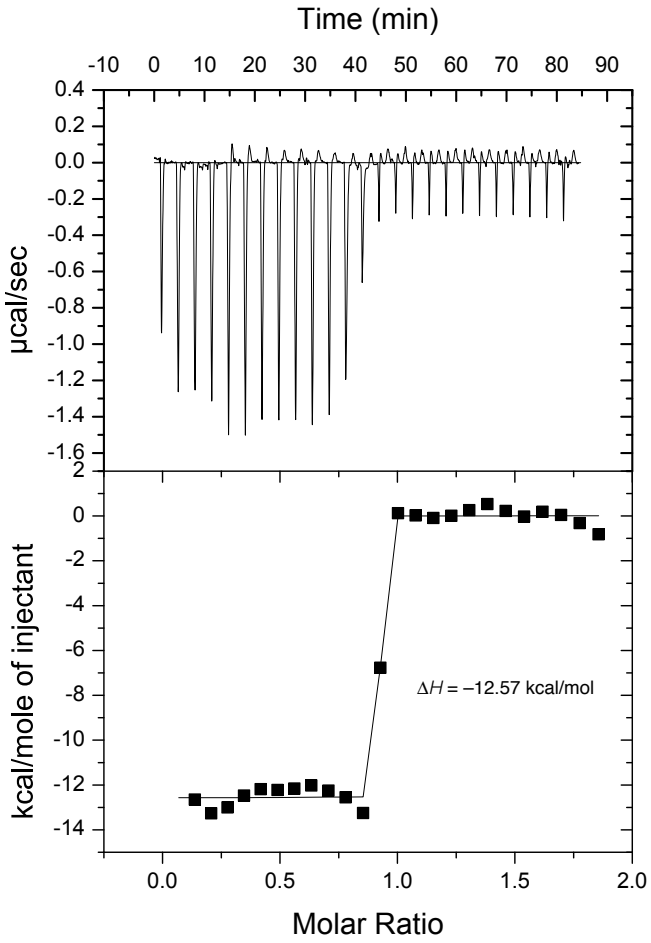

Fig. S2. Representative experimental data for ITC association analysis of (*P*)-(12,8)-[4]CC⊃**1** with hexyl substitutents in dichloromethane. Titration raw data (top), and curve analysis from ORIGIN program of the instrument (below). The titration experiments were run in triplicate, and the association enthalpy of –12.5±0.2 kcal/mol was obtained as the average.

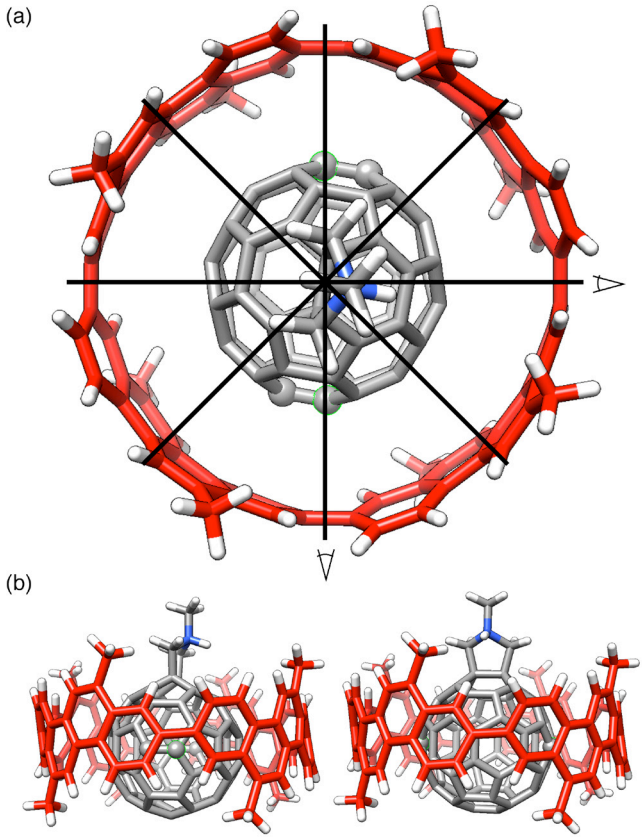

Fig. S3. Molecular structures of (*P*)-(12,8)-[4]CC⊃**1**$^+$ for the global minimum during the idealized single-axis rolling motions (0°, Fig. 3). Four carbon atoms on the equator of C_{60} moiety is shown in ball models, and, among them, two carbon atoms that are on the C_2 symmetry axis of [4]CC are highlighted with green fringes. (a) Top view. Black lines show the C_2 symmetry axis of [4]CC. (b) Side views.

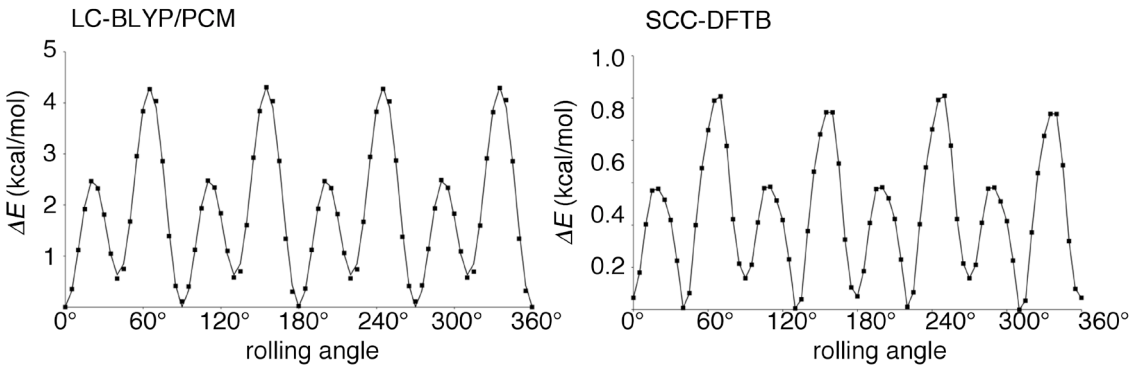

Fig. S4. Comparison of rolling energetics of (*P*)-(12,8)-[4]CC⊃**1**$^+$ by LC-BLYP/PCM and SCC-DFTB methods.

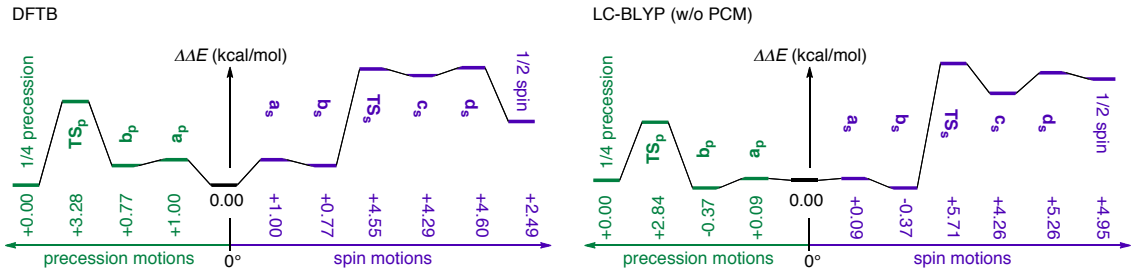

Fig. S5. Energy profiles from TS analysis. A profile from SCC-DFTB calculations through GRRM analysis is shown on the left, and a profile from single-point calculations (LC-BLYP/6-311G(d)//SCC-DFTB) is shown on the right.

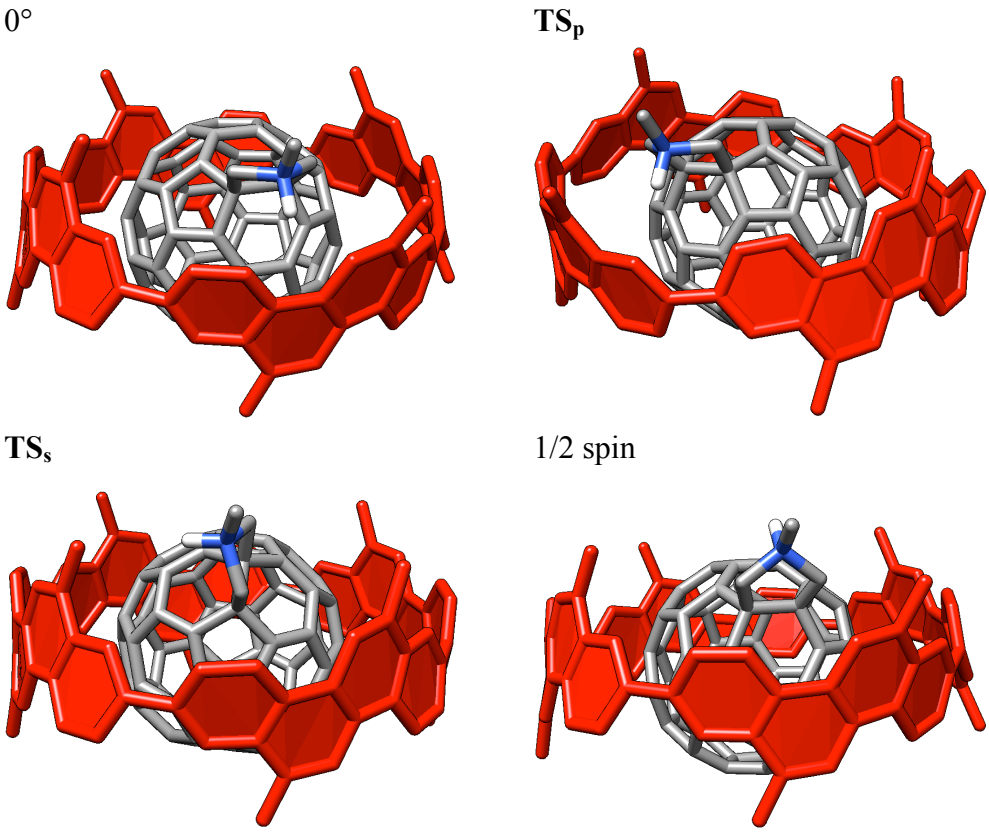

Fig. S6. Representative molecular structures from TS analysis shown in Fig. S5 and 4c.

Supporting Tables

Table S1. Comparison of association energies by other functionals and basis sets through single-point calculations[a,b,1]

Methods	ΔE with PCM	Deviation[c]
experiment (ΔH)	–12.5	—
LC-BLYP/6-311G(d)/PCM	–9.2	+3.3
LC-BLYP/6-311G(d,p)/PCM [d]	–9.6	+2.9
BLYP/6-311G(d)/PCM [e]	+30.2	+42.7
B3LYP/6-311G(d)/PCM [e]	+20.7	+33.2
TPSS/6-311G(d)/PCM [e]	+13.5	+26.0
PBE/6-311G(d)/PCM [e]	+5.5	+18.0
PBE0/6-311G(d)/PCM [e]	+2.2	+14.7
BLYP-D3/6-311G(d)/PCM [e]	–55.6	–43.1
B3LYP-D3/6-311G(d)/PCM [e]	–51.8	–39.3
TPSS-D3/6-311G(d)/PCM [e]	–53.1	–40.6
PBE-D3/6-311G(d)/PCM [e]	–48.1	–35.6
PBE0-D3/6-311G(d)/PCM [e]	–50.8	–38.3

[a] The geometry from LC-BLYP/PCM/6-311G(d) was used. [b] Data are shown in kcal/mol. [c] Deviation from the experimental value. The value from DFT calculations with PCM solvation was subtracted by the experimental value of –12.5 kcal/mol. [d] The value of BSSE corrections were also obtained with LC-BLYP/6-311G(d,p).[e] The value of BSSE corrections from LC-BLYP/6-311G(d) (Table S3) was applied.

1 For B3LYP: A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652. For BLYP: A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100; C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B,* 1988, **37**, 785-789. For PBE: J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865-3868. For PBE0: C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158-6169. For TPSS: J. M. Tao, J. P. Perdew, V. N. Staroverov and G. E. Scuseria, *Phys. Rev. Lett.*, 2003, **91**, 146401. For dispersion treatment with GD3: S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.

Table S2. Comparison of theoretical energetics of (*P*)-(12,8)-[4]CC⊃**1** and (*P*)-(12,8)-[4]CC⊃$\mathbf{1}^+$ by DFT methods[a]

Methods	ΔE (**1**) (kcal/mol)	ΔE ($\mathbf{1}^+$) (kcal/mol)	ΔE ($\mathbf{1}^+$)–ΔE (**1**) (kcal/mol)
CAM-B3LYP/PCM	+7.6	+6.7	–0.9
LC-BOP/PCM	+4.3	+3.5	–0.7
LC-ωPBE/PCM	–1.3	–2.1	–0.8
BMK/PCM	–7.6	–8.5	–0.9
LC-BLYP/PCM	–9.2	–10.1	–0.9
ωB97X/PCM	–25.0	–25.8	–0.8
ωB97/PCM	–32.9	–33.7	–0.8
M06-2X/PCM	–44.5	–45.3	–0.8
B97-D/PCM	–59.2	–60.7	–1.5
ωB97X-D/PCM	–66.6	–67.4	–0.8

[a] The basis set of 6-311G(d) was commonly used.

Table S3. Energy corrections (ΔE_c) for BSSE with the counterpoise method.

Methods	ΔE_c (kcal/mol)
CAM-B3LYP	+7.7
LC-BOP	+7.9
LC-ωPBE	+8.3
BMK	+7.9
LC-BLYP	+8.3
ωB97X	+6.9
ωB97	+6.6
M06-2X	+9.9
B97-D	+9.5
ωB97X-D	+8.9

Table S4. Event counts of precession and spin motions accumulated for 4000 ps

MD temperature	count	
	precession	spin
400 K	53	13
500 K	154	67
600 K	294	100
700 K	467	237

Table S5. Rate constants of precession and spin motions in MD simulations

MD temperature	rate constant (s^{-1})	
	precession	spin
400 K	1.33×10^{10}	0.325×10^{10}
500 K	3.85×10^{10}	1.68×10^{10}
600 K	7.35×10^{10}	7.35×10^{10}
700 K	11.7×10^{10}	5.93×10^{10}

Representative Coordinates

Geometry optimized structure of (*P*)-(12,8)-[4]CC⊃**1** with LC-BLYP/6-311G(d) (Fig. 2 and S1)

C	-6.876338	1.012064	0.015537
C	-6.514927	1.778368	1.087840
C	-6.005201	3.078938	0.949117
C	-5.824266	3.608113	-0.330250
C	-6.395821	2.896649	-1.402372
C	-6.910629	1.651136	-1.237496
C	-5.527029	3.807492	2.088071
C	-4.928739	4.722735	-0.512533
C	-4.323019	5.290507	0.591862
C	-4.737525	4.876456	1.889926
C	-3.155585	6.113568	0.410884
C	-2.613447	6.261741	-0.866718
C	-3.374538	5.839684	-2.005879
C	-4.491992	5.117882	-1.808978
H	-6.485462	1.334470	2.072795
H	-6.383175	3.318488	-2.398528
H	-7.300506	1.127442	-2.101779
H	-4.346908	5.391071	2.758162
H	-5.028447	4.760796	-2.678586
C	-1.272625	6.662045	-1.000147
H	-0.827189	6.595862	-1.983065
C	-2.408936	6.630442	1.487040
H	-2.837679	6.657693	2.479853
C	-0.484179	6.948085	0.078022
C	-1.126014	7.040864	1.327916
H	-0.577297	7.393495	2.192583
C	0.993020	6.880807	-0.029651
C	1.743168	6.521104	1.054163

C	1.649118	6.912733	-1.273574
C	3.045519	6.010330	0.934812
H	1.283625	6.491883	2.032136
C	2.896941	6.398015	-1.419940
H	1.136935	7.300835	-2.145553
C	3.594319	5.829865	-0.336665
C	3.756025	5.531533	2.084681
H	3.333048	6.384164	-2.409901
C	4.718590	4.943768	-0.502066
C	4.830224	4.745277	1.902158
C	5.268832	4.337447	0.610440
C	5.143622	4.516453	-1.792285
H	5.330495	4.352878	2.777950
C	6.099592	3.174043	0.440348
C	5.871660	3.401883	-1.980198
H	4.803602	5.056881	-2.666255
C	6.272223	2.635863	-0.836140
C	6.604488	2.428682	1.522684
C	6.682628	1.297487	-0.965664
H	6.614431	2.855883	2.516476
C	7.025446	1.148677	1.367258
H	6.635731	0.854248	-1.950750
C	6.953870	0.507830	0.115856
H	7.367720	0.601192	2.236708
C	-6.946005	-0.463614	0.145738
C	-6.677884	-1.270909	-0.923484
C	-7.014195	-1.083799	1.407676
C	-6.267149	-2.607056	-0.773175
H	-6.633822	-0.843941	-1.915879
C	-6.592553	-2.360995	1.582879
H	-7.354363	-0.522186	2.268916
C	-6.090398	-3.123877	0.511524
C	-5.870121	-3.392090	-1.905518

H	-6.599802	-2.772063	2.583463
C	-5.258310	-4.283722	0.698536
C	-5.141701	-4.503549	-1.701223
C	-4.712182	-4.909074	-0.405436
C	-4.813450	-4.667427	1.995431
H	-4.804416	-5.058525	-2.567111
C	-3.587085	-5.792002	-0.228986
C	-3.737362	-5.448812	2.187452
H	-5.309181	-4.258646	2.866263
C	-3.032499	-5.948790	1.043149
C	-2.894439	-6.379942	-1.304776
C	-1.729537	-6.457107	1.166023
H	-3.335030	-6.384332	-2.292856
C	-1.645954	-6.891999	-1.154533
H	-1.265522	-6.408799	2.141113
C	-0.984463	-6.837303	0.085734
H	-1.137494	-7.296090	-2.021448
C	6.884374	-0.969796	0.009822
C	6.526197	-1.718612	1.095459
C	6.915085	-1.629063	-1.232788
C	6.016360	-3.021355	0.979387
H	6.499549	-1.258824	2.073184
C	6.399992	-2.877163	-1.375887
H	7.302355	-1.119476	-2.106628
C	5.831674	-3.571226	-0.290712
C	5.541610	-3.731282	2.131399
H	6.384451	-3.315159	-2.365007
C	4.935858	-4.688820	-0.452265
C	4.751820	-4.803470	1.952939
C	4.333620	-5.238667	0.663013
C	4.494982	-5.104899	-1.740775
H	4.363523	-5.303761	2.830514
C	3.165662	-6.064574	0.499145

C	3.376860	-5.829723	-1.922340
H	5.028706	-4.762102	-2.617797
C	2.619242	-6.233195	-0.774104
C	2.422571	-6.563564	1.586058
C	1.277869	-6.635251	-0.896626
H	2.854250	-6.574339	2.577890
C	1.139052	-6.976072	1.437890
H	0.828929	-6.584895	-1.878925
C	0.493084	-6.903344	0.188853
H	0.592925	-7.313735	2.310106
C	-3.237312	-5.740140	3.565642
H	-2.298725	-5.219413	3.769277
H	-3.057117	-6.806102	3.713673
H	-3.958113	-5.415934	4.314707
C	-5.851695	3.339341	3.469918
H	-5.344517	2.400174	3.703281
H	-6.922019	3.170582	3.598679
H	-5.537310	4.072882	4.210787
C	-2.881141	6.127175	-3.386525
H	-1.989640	5.539107	-3.618770
H	-2.620327	7.179019	-3.513243
H	-3.638055	5.877972	-4.128571
C	3.264498	5.851589	3.459599
H	2.323473	5.341041	3.677507
H	3.090828	6.921160	3.588128
H	3.987159	5.537712	4.211285
C	6.190087	2.916291	-3.357062
H	5.611164	2.023603	-3.606777
H	7.245512	2.660582	-3.462904
H	5.953431	3.676047	-4.100316
C	5.869994	-3.240547	3.504527
H	5.364579	-2.296911	3.723406
H	6.940795	-3.070817	3.628046

H	5.556587	-3.961389	4.258172
C	2.879113	-6.139648	-3.296541
H	1.986865	-5.555373	-3.535365
H	2.617838	-7.193394	-3.405202
H	3.633659	-5.902631	-4.044977
C	-6.192629	-2.929403	-3.289318
H	-5.614551	-2.040931	-3.555538
H	-7.248401	-2.675582	-3.396367
H	-5.958014	-3.701363	-4.020552
C	1.235200	2.053487	1.908162
C	-0.200551	2.388170	1.908846
C	-1.113467	1.487727	2.340575
C	1.656943	0.842437	2.340329
C	1.812847	2.643476	0.737524
C	0.776887	3.336279	0.016725
C	-0.458413	3.173606	0.738086
C	-1.636768	3.030471	0.049437
C	-2.321395	1.308447	1.603819
C	-1.635278	-0.780666	2.350543
C	-1.221386	-1.997373	1.933173
C	0.213116	-2.331772	1.933328
C	1.121784	-1.422849	2.349709
C	2.330411	-1.253882	1.610523
C	2.661040	0.148547	1.603022
C	3.242443	0.710639	0.493778
C	2.807829	1.996050	0.049005
C	0.779160	3.347040	-1.350405
C	1.814163	2.651152	-2.073446
C	2.801190	1.993218	-1.391134
C	3.240311	0.695745	-1.836014
C	3.512185	-0.101711	-0.667520
C	3.200611	-1.430300	-0.659693
C	2.601010	-2.026261	0.509146

C	1.644556	-2.993989	0.077025
C	0.468248	-3.129417	0.770514
C	-2.645089	-0.095604	1.611633
C	-1.812453	-2.637829	-2.039913
C	-2.797194	-1.972193	-1.361635
C	-3.237527	-0.679503	-1.819175
C	-2.671405	-0.116327	-2.932780
C	-1.636103	-0.817782	-3.646340
C	0.186391	-2.375120	-3.210417
C	0.459334	-3.168113	-2.040943
C	-0.775392	-3.326082	-1.312515
C	-0.769142	-3.300425	0.054597
C	-1.802794	-2.599295	0.770752
C	-2.799876	-1.959617	0.078258
C	-3.505312	0.130544	-0.658205
C	-3.195687	1.459584	-0.666495
C	-2.599478	2.054043	-1.834686
C	-2.344339	1.288275	-2.940803
C	-1.106871	1.452568	-3.658973
C	-0.669007	0.151133	-4.096962
C	0.664907	-0.159446	-4.097208
C	1.104103	-1.455963	-3.646722
C	1.636418	-3.003377	-1.362554
C	2.601685	-2.037662	-1.820036
C	2.343569	-1.283835	-2.933590
C	2.670789	0.120726	-2.941846
C	1.633291	0.814397	-3.659600
C	1.217012	2.049105	-3.234878
C	-0.187926	2.376469	-3.235611
C	-0.457613	3.181388	-2.073651
C	-1.632877	3.024488	-1.390410
C	-3.231744	-0.669407	0.511026
C	-2.593244	2.068179	0.494114

C	-1.218492	-2.047750	-3.209152
C	0.780920	-0.141548	3.088930
C	1.106768	-0.234581	4.584889
H	1.892019	-0.961956	4.794044
C	-0.762538	0.218102	3.089241
C	-1.095025	0.279411	4.585352
H	-0.962889	1.312468	4.951422
H	-2.121051	-0.024903	4.795194
N	-0.141997	-0.611573	5.187791
C	-0.136264	-0.588441	6.622545
H	-1.111116	-0.890712	7.005756
H	0.604113	-1.291190	7.005352
H	0.097238	0.411238	7.024327
H	1.446044	0.749981	4.951219

Geometry optimized structure of (*P*)-(12,8)-[4]CC⊃**1** with CAM-B3LYP/6-311G(d) (Fig. S1)

C	-6.931251	1.040444	0.179351
C	-6.572585	1.819399	1.260969
C	-6.057314	3.124827	1.125274
C	-5.869888	3.662188	-0.167081
C	-6.443103	2.944391	-1.242738
C	-6.959666	1.686412	-1.078536
C	-5.580610	3.855983	2.270042
C	-4.969487	4.782272	-0.345686
C	-4.342706	5.337598	0.773460
C	-4.767201	4.922632	2.072402
C	-3.164166	6.155113	0.591901
C	-2.633522	6.333469	-0.703812
C	-3.429542	5.953658	-1.841861
C	-4.552588	5.217017	-1.640949
H	-6.552623	1.379433	2.247897
H	-6.422342	3.361137	-2.241641

H	-7.339890	1.163276	-1.947995
H	-4.374846	5.433095	2.943125
H	-5.110358	4.891224	-2.510435
C	-1.284172	6.729245	-0.846771
H	-0.855490	6.691810	-1.839116
C	-2.393093	6.645956	1.670815
H	-2.804015	6.652181	2.672101
C	-0.466964	6.982432	0.236260
C	-1.099092	7.053228	1.500721
H	-0.539827	7.382201	2.368157
C	1.016871	6.907671	0.118336
C	1.782524	6.559161	1.212558
C	1.677379	6.926271	-1.131744
C	3.091666	6.047997	1.097546
H	1.329067	6.543923	2.193539
C	2.939672	6.414309	-1.275963
H	1.162953	7.295936	-2.010877
C	3.648516	5.856565	-0.186272
C	3.808748	5.580845	2.255255
H	3.368724	6.386978	-2.269439
C	4.783189	4.970809	-0.343886
C	4.885034	4.775868	2.076806
C	5.326002	4.352867	0.785927
C	5.245303	4.556454	-1.630277
H	5.384118	4.389524	2.956771
C	6.157748	3.182113	0.621120
C	5.993947	3.438991	-1.816291
H	4.928955	5.108987	-2.506507
C	6.361693	2.649117	-0.669964
C	6.640153	2.419511	1.709931
C	6.772660	1.302968	-0.801885
H	6.628747	2.834427	2.709532
C	7.060884	1.128492	1.550571

H	6.755044	0.870953	-1.793299
C	7.013008	0.490846	0.287837
H	7.381181	0.575383	2.425128
C	-7.005868	-0.441928	0.316988
C	-6.768653	-1.273187	-0.758915
C	-7.050731	-1.057157	1.590888
C	-6.357509	-2.616928	-0.604338
H	-6.753638	-0.858747	-1.757872
C	-6.629434	-2.345105	1.771868
H	-7.369168	-0.488741	2.456280
C	-6.149576	-3.126682	0.695435
C	-5.993270	-3.427385	-1.737351
H	-6.615735	-2.742614	2.778481
C	-5.316464	-4.293672	0.878862
C	-5.244270	-4.541529	-1.533425
C	-4.777685	-4.932395	-0.241279
C	-4.869127	-4.690634	2.175760
H	-4.930778	-5.109894	-2.400522
C	-3.641967	-5.814619	-0.071415
C	-3.790646	-5.490091	2.365135
H	-5.363797	-4.286740	3.050291
C	-3.079149	-5.980042	1.213440
C	-2.937552	-6.393377	-1.153020
C	-1.769283	-6.488222	1.332736
H	-3.370950	-6.385763	-2.144976
C	-1.674400	-6.902073	-1.004276
H	-1.311406	-6.452220	2.311077
C	-1.008561	-6.858880	0.242361
H	-1.163568	-7.288768	-1.878196
C	6.938982	-0.993749	0.176217
C	6.584186	-1.754027	1.272292
C	6.963599	-1.661309	-1.070407
C	6.069049	-3.061796	1.160837

H	6.567269	-1.297098	2.251548
C	6.447050	-2.922152	-1.211154
H	7.340708	-1.153174	-1.950061
C	5.877574	-3.621456	-0.121442
C	5.596098	-3.773089	2.319544
H	6.423112	-3.356078	-2.202643
C	4.976885	-4.744645	-0.277871
C	4.781924	-4.842805	2.142888
C	4.353400	-5.280197	0.852636
C	4.556263	-5.202278	-1.564054
H	4.392156	-5.338074	3.023471
C	3.174163	-6.100476	0.689019
C	3.432724	-5.942493	-1.748584
H	5.111699	-4.892273	-2.440793
C	2.639673	-6.301790	-0.601752
C	2.406104	-6.571282	1.778869
C	1.289727	-6.699539	-0.733710
H	2.819506	-6.559030	2.779049
C	1.111491	-6.980859	1.619891
H	0.857940	-6.679651	-1.725264
C	0.475663	-6.932452	0.356272
H	0.554439	-7.293056	2.494867
C	-3.303804	-5.802805	3.752649
H	-2.357990	-5.299280	3.973278
H	-3.140611	-6.874015	3.893023
H	-4.027996	-5.475192	4.498850
C	-5.925743	3.403563	3.661576
H	-5.442299	2.454502	3.911714
H	-7.001698	3.259185	3.785190
H	-5.600760	4.138250	4.398600
C	-2.980416	6.302164	-3.232665
H	-2.086696	5.739763	-3.519105
H	-2.739778	7.363773	-3.326117

H	-3.757709	6.069725	-3.960825
C	3.331134	5.925107	3.638541
H	2.382594	5.433646	3.874524
H	3.175693	7.000059	3.757498
H	4.056820	5.608097	4.387852
C	6.367576	2.988419	-3.200447
H	5.815967	2.090361	-3.494196
H	7.432113	2.754736	-3.276756
H	6.141456	3.762413	-3.934074
C	5.946154	-3.297058	3.701970
H	5.465559	-2.342661	3.937039
H	7.022742	-3.152546	3.819888
H	5.622078	-4.018220	4.452635
C	2.980097	-6.316435	-3.131633
H	2.085630	-5.759442	-3.426105
H	2.739325	-7.379599	-3.204882
H	3.755549	-6.097398	-3.865900
C	-6.371591	-3.002095	-3.128243
H	-5.822215	-2.108760	-3.440068
H	-7.436690	-2.771183	-3.205446
H	-6.146746	-3.788897	-3.848520
C	1.170660	2.097095	1.597360
C	-0.279977	2.384402	1.598819
C	-1.172268	1.446408	2.033267
C	1.639132	0.889809	2.031155
C	1.730230	2.711280	0.421433
C	0.667456	3.371988	-0.301073
C	-0.565345	3.166291	0.423541
C	-1.748156	2.984204	-0.273098
C	-2.375639	1.225673	1.288761
C	-1.621165	-0.851797	2.036216
C	-1.159971	-2.062093	1.609400
C	0.289643	-2.349173	1.608369

C	1.177797	-1.405911	2.033508
C	2.381911	-1.190619	1.287646
C	2.666280	0.227670	1.284629
C	3.232629	0.816586	0.165776
C	2.753927	2.093498	-0.276752
C	0.669814	3.389061	-1.681583
C	1.732466	2.729799	-2.411142
C	2.749614	2.096693	-1.722668
C	3.233678	0.810103	-2.174152
C	3.531888	0.015499	-1.002721
C	3.263178	-1.335374	-0.999208
C	2.681843	-1.956330	0.172783
C	1.753349	-2.957153	-0.264518
C	0.572433	-3.135778	0.435978
C	-2.653567	-0.193893	1.292175
C	-1.732794	-2.712976	-2.394662
C	-2.747826	-2.076337	-1.706101
C	-3.233043	-0.791726	-2.162091
C	-2.681785	-0.201050	-3.285364
C	-1.619542	-0.868516	-4.005331
C	0.264901	-2.378847	-3.569754
C	0.565177	-3.168376	-2.396699
C	-0.668231	-3.369085	-1.665028
C	-0.662191	-3.345346	-0.284426
C	-1.722874	-2.680945	0.437793
C	-2.748440	-2.066597	-0.260457
C	-3.527439	0.008244	-0.993095
C	-3.260550	1.359465	-0.997148
C	-2.683801	1.980343	-2.168888
C	-2.400620	1.219996	-3.288702
C	-1.164273	1.428900	-4.010521
C	-0.681214	0.138259	-4.454871
C	0.675632	-0.130328	-4.456048

C	1.159912	-1.418823	-4.007414
C	1.746887	-2.964864	-1.709697
C	2.684046	-1.961901	-2.167014
C	2.398088	-1.206556	-3.289462
C	2.679320	0.214469	-3.293326
C	1.615114	0.878604	-4.013208
C	1.153672	2.109435	-3.580321
C	-0.268152	2.390945	-3.579805
C	-0.565435	3.185224	-2.409263
C	-1.745470	2.985262	-1.718546
C	-3.224722	-0.787692	0.178187
C	-2.676617	1.985755	0.170520
C	-1.156893	-2.097335	-3.567821
C	0.792923	-0.131703	2.782800
C	1.123074	-0.214020	4.291404
H	1.927434	-0.921230	4.500071
C	-0.778199	0.179466	2.784134
C	-1.112146	0.229484	4.293291
H	-1.024486	1.269791	4.655543
H	-2.125283	-0.116848	4.503729
N	-0.120726	-0.630830	4.901405
C	-0.113269	-0.599594	6.345600
H	-1.078344	-0.934085	6.729863
H	0.651577	-1.277406	6.728345
H	0.087232	0.408924	6.747500
H	1.440081	0.780646	4.653731

Geometry optimized structure of (*P*)-(12,8)-[4]CC⊃**1** with LC-BOP/6-311G(d) (Fig. S1)

C	-6.886282	1.014849	0.058520
C	-6.529376	1.786125	1.131605
C	-6.023491	3.091043	0.995818
C	-5.841572	3.624882	-0.283398

C	-6.410491	2.909135	-1.356892
C	-6.920202	1.658801	-1.194468
C	-5.553189	3.823447	2.138959
C	-4.949636	4.747632	-0.461452
C	-4.337977	5.307233	0.645639
C	-4.758249	4.890817	1.943338
C	-3.166519	6.130379	0.466054
C	-2.634381	6.299231	-0.814818
C	-3.416803	5.906129	-1.953912
C	-4.528855	5.172495	-1.756531
H	-6.503833	1.345422	2.117685
H	-6.398537	3.329741	-2.353663
H	-7.305674	1.137379	-2.062102
H	-4.374974	5.408278	2.813027
H	-5.081408	4.839775	-2.625733
C	-1.289477	6.695517	-0.953955
H	-0.856284	6.647768	-1.943288
C	-2.406403	6.630946	1.542920
H	-2.824684	6.648199	2.540399
C	-0.485978	6.958700	0.122016
C	-1.121669	7.038548	1.378457
H	-0.568716	7.379249	2.245016
C	0.996103	6.888476	0.007831
C	1.754426	6.537584	1.091756
C	1.653946	6.916091	-1.237736
C	3.061069	6.031076	0.973708
H	1.300894	6.515271	2.072243
C	2.906458	6.406695	-1.383110
H	1.141800	7.296330	-2.113177
C	3.611354	5.845583	-0.298329
C	3.778653	5.564310	2.127542
H	3.338661	6.390185	-2.374823
C	4.743919	4.963429	-0.459339

C	4.851516	4.773025	1.947407
C	5.289685	4.355491	0.656289
C	5.194471	4.547552	-1.747363
H	5.357050	4.391225	2.824729
C	6.120892	3.188037	0.489410
C	5.934538	3.438211	-1.933712
H	4.874948	5.100259	-2.621395
C	6.310656	2.655567	-0.788661
C	6.611978	2.432585	1.573580
C	6.716347	1.312553	-0.920408
H	6.614580	2.852655	2.570447
C	7.028715	1.149835	1.416206
H	6.685035	0.878050	-1.909890
C	6.966901	0.511259	0.160580
H	7.360621	0.600438	2.288315
C	-6.959169	-0.465764	0.191955
C	-6.711905	-1.284986	-0.876289
C	-7.017347	-1.083228	1.458249
C	-6.305562	-2.625611	-0.723297
H	-6.683742	-0.867121	-1.873031
C	-6.599669	-2.363000	1.635786
H	-7.347152	-0.519447	2.321951
C	-6.111280	-3.136212	0.562965
C	-5.932961	-3.427577	-1.856062
H	-6.599426	-2.766604	2.639422
C	-5.278393	-4.299861	0.747088
C	-5.192181	-4.533573	-1.653194
C	-4.736844	-4.927192	-0.359840
C	-4.833435	-4.692474	2.043610
H	-4.875373	-5.100991	-2.518759
C	-3.603333	-5.806057	-0.187781
C	-3.758443	-5.478579	2.233409
H	-5.334079	-4.293791	2.916174

C	-3.046906	-5.967217	1.084935
C	-2.903386	-6.387438	-1.265133
C	-1.739623	-6.471231	1.206345
H	-3.340260	-6.389606	-2.254949
C	-1.650211	-6.894193	-1.116043
H	-1.281353	-6.429192	2.183964
C	-0.986670	-6.843279	0.125767
H	-1.142035	-7.290898	-1.986509
C	6.894367	-0.971393	0.051766
C	6.541485	-1.725112	1.138553
C	6.924261	-1.635713	-1.190630
C	6.035892	-3.032346	1.025921
H	6.519090	-1.268354	2.117383
C	6.414624	-2.888782	-1.330770
H	7.306461	-1.128467	-2.068061
C	5.849794	-3.587147	-0.243763
C	5.569852	-3.746089	2.182484
H	6.399323	-3.325652	-2.320473
C	4.957833	-4.713079	-0.400384
C	4.774580	-4.816691	2.007055
C	4.349997	-5.254417	0.717791
C	4.532636	-5.159251	-1.686865
H	4.394217	-5.319839	2.886348
C	3.177827	-6.080237	0.555876
C	3.419778	-5.895817	-1.868239
H	5.082327	-4.841188	-2.563355
C	2.641068	-6.269912	-0.720168
C	2.421348	-6.562250	1.643612
C	1.295503	-6.667827	-0.848039
H	2.842711	-6.562545	2.639918
C	1.135856	-6.971735	1.490468
H	0.858617	-6.636315	-1.836436
C	0.495794	-6.912448	0.235167

H	0.585568	-7.296833	2.364647
C	-3.270945	-5.789677	3.615019
H	-2.334840	-5.272032	3.836418
H	-3.094011	-6.858007	3.749550
H	-3.999431	-5.476424	4.361356
C	-5.895956	3.366284	3.523399
H	-5.394194	2.428425	3.772481
H	-6.968535	3.202870	3.640068
H	-5.589429	4.105587	4.261879
C	-2.959175	6.248881	-3.337610
H	-2.068435	5.681066	-3.616256
H	-2.713930	7.308113	-3.429861
H	-3.732298	6.020235	-4.069542
C	3.300662	5.905674	3.505361
H	2.361545	5.400197	3.741818
H	3.131827	6.977683	3.619574
H	4.030817	5.602105	4.254081
C	6.302487	2.982832	-3.311881
H	5.742579	2.090650	-3.601717
H	7.363939	2.741084	-3.386287
H	6.084003	3.756091	-4.046773
C	5.917433	-3.266343	3.558074
H	5.417938	-2.323615	3.793048
H	6.990588	-3.102449	3.668749
H	5.612245	-3.992872	4.309676
C	2.957201	-6.261004	-3.244526
H	2.066066	-5.696856	-3.529320
H	2.710560	-7.321344	-3.318410
H	3.728049	-6.045264	-3.982763
C	-6.305489	-2.995784	-3.240598
H	-5.747069	-2.108327	-3.547348
H	-7.367334	-2.755953	-3.315796
H	-6.088814	-3.781267	-3.962960

C	1.237501	2.050305	1.820382
C	-0.198441	2.387519	1.820625
C	-1.113496	1.487609	2.252375
C	1.657319	0.837603	2.253018
C	1.815897	2.638840	0.648172
C	0.781190	3.333015	-0.073777
C	-0.454468	3.172543	0.648071
C	-1.632646	3.031460	-0.042364
C	-2.321384	1.310348	1.513138
C	-1.639186	-0.781121	2.261144
C	-1.226662	-1.998893	1.842080
C	0.208035	-2.335800	1.842714
C	1.118605	-1.428075	2.261248
C	2.327741	-1.260228	1.520608
C	2.660692	0.142184	1.514052
C	3.242262	0.703650	0.403361
C	2.809917	1.990063	-0.041409
C	0.784403	3.345563	-1.442063
C	1.819401	2.649569	-2.166309
C	2.804750	1.988811	-1.482498
C	3.242331	0.690468	-1.928493
C	3.511641	-0.107961	-0.759210
C	3.198177	-1.436652	-0.752288
C	2.597097	-2.031795	0.416956
C	1.639066	-2.997559	-0.016674
C	0.462346	-3.131665	0.677400
C	-2.647483	-0.093672	1.520198
C	-1.817230	-2.636632	-2.137366
C	-2.800868	-1.968884	-1.457722
C	-3.239254	-0.674809	-1.915320
C	-2.672576	-0.111806	-3.030231
C	-1.637817	-0.815157	-3.745023
C	0.183488	-2.376721	-3.308400

C	0.454603	-3.170014	-2.137371
C	-0.780776	-3.325725	-1.408598
C	-0.774747	-3.299698	-0.040322
C	-1.807758	-2.598021	0.676856
C	-2.803277	-1.956271	-0.016895
C	-3.505452	0.134937	-0.752910
C	-3.193937	1.464085	-0.760364
C	-2.597277	2.058716	-1.929197
C	-2.343227	1.293150	-3.037369
C	-1.104586	1.456180	-3.756125
C	-0.668262	0.153269	-4.195430
C	0.666467	-0.159687	-4.195259
C	1.103740	-1.458178	-3.744502
C	1.632002	-3.007199	-1.457182
C	2.599796	-2.042893	-1.914481
C	2.343746	-1.288077	-3.029494
C	2.673236	0.116844	-3.036773
C	1.636902	0.813182	-3.755913
C	1.221994	2.049331	-3.330076
C	-0.183500	2.378996	-3.331099
C	-0.452386	3.182982	-2.166948
C	-1.628563	3.027286	-1.483145
C	-3.233256	-0.665570	0.416923
C	-2.591045	2.070575	0.401859
C	-1.221969	-2.047057	-3.307737
C	0.779457	-0.146029	3.003863
C	1.106501	-0.239031	4.502227
H	1.888051	-0.970385	4.710910
C	-0.765116	0.216450	3.003647
C	-1.099559	0.279453	4.501920
H	-0.971896	1.313341	4.865734
H	-2.125132	-0.026994	4.710548
N	-0.145075	-0.611455	5.107377

C	-0.140625	-0.591792	6.544932
H	-1.116321	-0.895025	6.925377
H	0.597715	-1.297932	6.925576
H	0.093625	0.404955	6.952551
H	1.452808	0.743365	4.866300

Geometry optimized structure of (*P*)-(12,8)-[4]CC⊃**1** with LC-ωPBE/6-311G(d) (Fig. S1)

C	-6.901647	1.014778	0.024100
C	-6.532971	1.782762	1.102144
C	-6.025239	3.090241	0.964423
C	-5.847338	3.624840	-0.320842
C	-6.426100	2.912975	-1.396020
C	-6.943321	1.660469	-1.231359
C	-5.550208	3.823561	2.108314
C	-4.950233	4.745244	-0.503390
C	-4.339134	5.313509	0.606942
C	-4.756768	4.898992	1.909221
C	-3.167880	6.140378	0.424439
C	-2.626681	6.292649	-0.860744
C	-3.399231	5.881966	-2.003367
C	-4.521239	5.153474	-1.804011
H	-6.499084	1.336011	2.087788
H	-6.419735	3.337177	-2.392899
H	-7.339962	1.140731	-2.096796
H	-4.369731	5.416850	2.779210
H	-5.066605	4.807309	-2.674547
C	-1.279612	6.690938	-0.997191
H	-0.836368	6.626552	-1.983343
C	-2.416695	6.660813	1.502621
H	-2.843616	6.690969	2.497842
C	-0.484216	6.977139	0.085377
C	-1.127509	7.074116	1.340103

H	-0.579078	7.431127	2.205022
C	0.998336	6.909890	-0.025253
C	1.753785	6.548739	1.063738
C	1.657908	6.945862	-1.273402
C	3.062714	6.039460	0.943486
H	1.294618	6.519001	2.043964
C	2.912469	6.428795	-1.421095
H	1.147285	7.337675	-2.146449
C	3.612910	5.856741	-0.334761
C	3.781188	5.567763	2.097948
H	3.348422	6.418248	-2.412840
C	4.742337	4.968492	-0.500479
C	4.860551	4.775823	1.914203
C	5.295703	4.360023	0.618437
C	5.177042	4.545039	-1.794415
H	5.366316	4.389747	2.791710
C	6.129204	3.191796	0.448257
C	5.911683	3.425584	-1.983206
H	4.845644	5.091781	-2.669810
C	6.303371	2.651276	-0.834701
C	6.638693	2.444101	1.533727
C	6.711332	1.306283	-0.964783
H	6.653465	2.871915	2.528902
C	7.060631	1.156888	1.377497
H	6.664782	0.862932	-1.951960
C	6.982686	0.511830	0.122705
H	7.407743	0.611094	2.247994
C	-6.974242	-0.466255	0.154536
C	-6.706131	-1.278923	-0.920243
C	-7.049034	-1.090028	1.420202
C	-6.298039	-2.621686	-0.768635
H	-6.662315	-0.852266	-1.914903
C	-6.626494	-2.374356	1.596924

H	-7.394175	-0.529674	2.282209
C	-6.119684	-3.140079	0.522822
C	-5.910134	-3.415806	-1.904835
H	-6.638804	-2.785649	2.599064
C	-5.284650	-4.304501	0.710566
C	-5.175336	-4.532199	-1.699047
C	-4.735829	-4.933002	-0.399488
C	-4.842303	-4.694522	2.011824
H	-4.846922	-5.094070	-2.565959
C	-3.605456	-5.817888	-0.222417
C	-3.760631	-5.480942	2.205340
H	-5.342907	-4.290995	2.884390
C	-3.048608	-5.975221	1.056365
C	-2.910361	-6.410994	-1.300943
C	-1.738907	-6.481662	1.179851
H	-3.351468	-6.419990	-2.290443
C	-1.654981	-6.925088	-1.149539
H	-1.274580	-6.431415	2.156791
C	-0.989237	-6.864707	0.094382
H	-1.148558	-7.333921	-2.017250
C	6.910519	-0.971219	0.016984
C	6.545994	-1.721546	1.108759
C	6.947789	-1.637321	-1.227910
C	6.038035	-3.031185	0.994270
H	6.515708	-1.258846	2.087141
C	6.430182	-2.892411	-1.370186
H	7.341229	-1.131848	-2.103201
C	5.855382	-3.586676	-0.281456
C	5.567307	-3.745738	2.151674
H	6.420229	-3.332883	-2.359953
C	4.957817	-4.710008	-0.442449
C	4.773156	-4.824213	1.973031
C	4.350785	-5.259947	0.679242

C	4.524040	-5.139602	-1.734614
H	4.389103	-5.327669	2.852718
C	3.178753	-6.089506	0.514727
C	3.401301	-5.871249	-1.917766
H	5.066312	-4.808073	-2.612762
C	2.632665	-6.262783	-0.765747
C	2.431529	-6.591407	1.604280
C	1.284949	-6.662800	-0.890584
H	2.861756	-6.604529	2.598421
C	1.141650	-7.006846	1.453494
H	0.837706	-6.614596	-1.875898
C	0.493717	-6.930560	0.199787
H	0.596107	-7.348442	2.326393
C	-3.267866	-5.783629	3.589692
H	-2.333034	-5.258474	3.804769
H	-3.085057	-6.851772	3.727244
H	-3.997495	-5.469792	4.336417
C	-5.883112	3.359727	3.495663
H	-5.371021	2.424102	3.737534
H	-6.955111	3.187661	3.615902
H	-5.577523	4.100565	4.234767
C	-2.920624	6.193563	-3.390040
H	-2.031303	5.609095	-3.643113
H	-2.663345	7.249469	-3.499540
H	-3.687807	5.956363	-4.127230
C	3.298407	5.901654	3.478683
H	2.360866	5.388124	3.709710
H	3.123173	6.973557	3.595239
H	4.030243	5.598484	4.227674
C	6.251149	2.951183	-3.364982
H	5.675084	2.060495	-3.631911
H	7.309906	2.698047	-3.455060
H	6.025339	3.719502	-4.104569

C	5.905533	-3.259468	3.530041
H	5.396278	-2.318776	3.757950
H	6.978248	-3.087484	3.643971
H	5.600981	-3.987349	4.282335
C	2.917837	-6.206046	-3.297312
H	2.027610	-5.625847	-3.556906
H	2.660121	-7.263620	-3.388071
H	3.682409	-5.981333	-4.041109
C	-6.253680	-2.965052	-3.293520
H	-5.678186	-2.079240	-3.577443
H	-7.312649	-2.713188	-3.384798
H	-6.030259	-3.746002	-4.020500
C	1.237993	2.059532	1.900635
C	-0.200934	2.395676	1.900625
C	-1.118036	1.487623	2.330949
C	1.658832	0.839683	2.332143
C	1.818840	2.651388	0.727431
C	0.780416	3.346918	0.004249
C	-0.459050	3.184206	0.726961
C	-1.643081	3.041547	0.033450
C	-2.329355	1.310026	1.591461
C	-1.642001	-0.785729	2.338143
C	-1.228302	-2.010289	1.919383
C	0.209421	-2.346144	1.920285
C	1.121707	-1.430610	2.338712
C	2.334735	-1.261613	1.598901
C	2.666961	0.144809	1.593190
C	3.253825	0.710763	0.480086
C	2.819366	2.000996	0.035239
C	0.783755	3.359193	-1.370193
C	1.822204	2.662008	-2.095342
C	2.813372	1.999292	-1.409088
C	3.253236	0.698076	-1.856362

C	3.524874	-0.102892	-0.685286
C	3.211216	-1.438584	-0.679212
C	2.608498	-2.037415	0.491851
C	1.649622	-3.007703	0.056856
C	0.466571	-3.144127	0.753136
C	-2.654605	-0.098023	1.597525
C	-1.818610	-2.646659	-2.070434
C	-2.808503	-1.977721	-1.388224
C	-3.248937	-0.680292	-1.845963
C	-2.678983	-0.113121	-2.964475
C	-1.640573	-0.816382	-3.680247
C	0.187225	-2.382092	-3.242231
C	0.459665	-3.178967	-2.070222
C	-0.779161	-3.337767	-1.340875
C	-0.773880	-3.313565	0.033579
C	-1.811070	-2.611318	0.752125
C	-2.812725	-1.967210	0.055870
C	-3.518156	0.130673	-0.681008
C	-3.206496	1.466831	-0.687672
C	-2.607639	2.063976	-1.858113
C	-2.350552	1.295264	-2.970761
C	-1.108906	1.460358	-3.689919
C	-0.669916	0.155471	-4.130413
C	0.670799	-0.157201	-4.129994
C	1.110465	-1.458164	-3.679241
C	1.642524	-3.014763	-1.386967
C	2.611425	-2.046037	-1.844066
C	2.353015	-1.286816	-2.962858
C	2.681602	0.121527	-2.969233
C	1.642053	0.818595	-3.689195
C	1.223850	2.059363	-3.261102
C	-0.185087	2.388102	-3.262452
C	-0.456026	3.194304	-2.096579

C	-1.638101	3.036465	-1.410618
C	-3.245093	-0.673193	0.490907
C	-2.602621	2.075644	0.477399
C	-1.221668	-2.053345	-3.241742
C	0.779001	-0.146961	3.080888
C	1.105499	-0.240685	4.582667
H	1.891924	-0.969046	4.790276
C	-0.766562	0.213825	3.080380
C	-1.101526	0.275376	4.581943
H	-0.967658	1.309806	4.946874
H	-2.129519	-0.028556	4.789127
N	-0.148438	-0.625120	5.184099
C	-0.142164	-0.596410	6.625371
H	-1.118573	-0.899257	7.007315
H	0.598406	-1.300857	7.007836
H	0.091731	0.404113	7.027003
H	1.444141	0.745757	4.947906

Geometry optimized structure of (*P*)-(12,8)-[4]CC⊃**1** with BMK/6-311G(d) (Fig. S1)

C	-6.962231	1.029705	0.006595
C	-6.591508	1.800643	1.100341
C	-6.075352	3.113966	0.965246
C	-5.889169	3.653851	-0.337178
C	-6.474127	2.942851	-1.421536
C	-7.000797	1.682021	-1.257429
C	-5.596868	3.850591	2.114973
C	-4.981299	4.773290	-0.519509
C	-4.363006	5.346290	0.608539
C	-4.788592	4.931750	1.915714
C	-3.184485	6.174151	0.425910
C	-2.636823	6.328256	-0.877203
C	-3.410120	5.910672	-2.025702
C	-4.545208	5.178381	-1.825772

H	-6.564371	1.349081	2.084623
H	-6.463530	3.369631	-2.418475
H	-7.401595	1.165153	-2.123873
H	-4.396534	5.447060	2.786302
H	-5.084721	4.820759	-2.696593
C	-1.281934	6.727098	-1.013372
H	-0.836395	6.662958	-1.999005
C	-2.426466	6.693371	1.512011
H	-2.851683	6.719009	2.509218
C	-0.479330	7.013538	0.082184
C	-1.125256	7.107281	1.347521
H	-0.572185	7.458723	2.213198
C	1.007612	6.946270	-0.031559
C	1.772444	6.578015	1.066804
C	1.665697	6.982354	-1.292426
C	3.086085	6.059888	0.939451
H	1.314777	6.551817	2.048439
C	2.925917	6.452481	-1.449622
H	1.153376	7.382249	-2.161940
C	3.632407	5.870764	-0.360262
C	3.816322	5.583320	2.093872
H	3.357781	6.440512	-2.444304
C	4.762372	4.975147	-0.534892
C	4.903201	4.780950	1.901266
C	5.330918	4.360486	0.597004
C	5.182461	4.544457	-1.838282
H	5.413279	4.389157	2.775089
C	6.170759	3.189676	0.419680
C	5.920067	3.412604	-2.033594
H	4.828667	5.082381	-2.711558
C	6.334718	2.641443	-0.882242
C	6.695336	2.439317	1.508340
C	6.751044	1.291455	-1.014657

H	6.714300	2.866759	2.504742
C	7.124906	1.142645	1.346986
H	6.696060	0.844197	-1.999974
C	7.040816	0.493078	0.083231
H	7.479487	0.595478	2.215037
C	-7.033595	-0.456544	0.130437
C	-6.753047	-1.268057	-0.960144
C	-7.111673	-1.091123	1.402157
C	-6.337190	-2.617011	-0.814119
H	-6.703164	-0.831828	-1.950861
C	-6.682085	-2.386005	1.576254
H	-7.461352	-0.533490	2.265548
C	-6.163793	-3.148906	0.493345
C	-5.930265	-3.402811	-1.958353
H	-6.695606	-2.802125	2.577517
C	-5.320673	-4.315802	0.680022
C	-5.188586	-4.530428	-1.753616
C	-4.757620	-4.942913	-0.447720
C	-4.883239	-4.718115	1.986726
H	-4.840894	-5.079921	-2.622191
C	-3.623488	-5.832453	-0.268896
C	-3.792590	-5.514512	2.182746
H	-5.388025	-4.315868	2.858826
C	-3.068566	-6.003756	1.029759
C	-2.920840	-6.423818	-1.355469
C	-1.753028	-6.517378	1.155897
H	-3.357497	-6.423919	-2.348120
C	-1.658276	-6.948280	-1.199052
H	-1.290022	-6.478414	2.134601
C	-0.993591	-6.897162	0.057828
H	-1.149906	-7.356534	-2.066985
C	6.974512	-0.994700	-0.024362
C	6.620198	-1.757196	1.080588

C	7.002232	-1.658915	-1.282548
C	6.106348	-3.073222	0.963043
H	6.602720	-1.297081	2.061169
C	6.478673	-2.922991	-1.429199
H	7.392282	-1.149511	-2.158203
C	5.907012	-3.625529	-0.332197
C	5.640931	-3.800122	2.124301
H	6.459458	-3.358950	-2.422014
C	4.998675	-4.747754	-0.494991
C	4.828053	-4.881040	1.943216
C	4.387825	-5.306473	0.644305
C	4.552442	-5.168064	-1.793118
H	4.445471	-5.388416	2.822598
C	3.204907	-6.132362	0.480285
C	3.414076	-5.899467	-1.975911
H	5.085999	-4.824793	-2.673102
C	2.647493	-6.300034	-0.817019
C	2.451374	-6.633810	1.577764
C	1.290770	-6.695909	-0.939482
H	2.881704	-6.646834	2.572983
C	1.147277	-7.044157	1.426957
H	0.839601	-6.643341	-1.923140
C	0.493798	-6.965040	0.164497
H	0.598191	-7.380595	2.301034
C	-3.308528	-5.829035	3.582565
H	-2.363810	-5.317859	3.804678
H	-3.141291	-6.903517	3.717415
H	-4.042011	-5.504141	4.324997
C	-5.938011	3.389669	3.516297
H	-5.444239	2.440415	3.757594
H	-7.016497	3.238317	3.637310
H	-5.613947	4.128231	4.254084
C	-2.915538	6.198313	-3.426536

H	-2.023116	5.602720	-3.659807
H	-2.650089	7.253701	-3.552962
H	-3.681315	5.948836	-4.165397
C	3.343682	5.919695	3.492546
H	2.395931	5.419758	3.727083
H	3.185567	6.997122	3.614389
H	4.079207	5.598727	4.234693
C	6.217469	2.918281	-3.432738
H	5.627810	2.022390	-3.667751
H	7.274895	2.658662	-3.554288
H	5.967005	3.681992	-4.173400
C	6.000021	-3.328780	3.517640
H	5.509646	-2.377627	3.758390
H	7.080012	-3.176772	3.623459
H	5.685489	-4.061869	4.264954
C	2.908095	-6.200927	-3.369806
H	2.016331	-5.604155	-3.602875
H	2.637427	-7.256496	-3.482809
H	3.669268	-5.962627	-4.117085
C	-6.242500	-2.928914	-3.361361
H	-5.659150	-2.034003	-3.614766
H	-7.302142	-2.675250	-3.476234
H	-5.995971	-3.701792	-4.093803
C	1.195313	2.122513	1.950949
C	-0.257917	2.435331	1.938203
C	-1.174024	1.509063	2.377589
C	1.642913	0.903714	2.404375
C	1.779798	2.720277	0.767865
C	0.726569	3.395226	0.026292
C	-0.524098	3.217127	0.747195
C	-1.714967	3.043312	0.039561
C	-2.385815	1.299835	1.626674
C	-1.662598	-0.791415	2.406389

C	-1.216561	-2.023976	1.997662
C	0.235729	-2.336530	2.012103
C	1.141229	-1.394205	2.432186
C	2.364375	-1.209469	1.692408
C	2.673673	0.212605	1.673076
C	3.267402	0.784226	0.546268
C	2.807916	2.071784	0.081406
C	0.738919	3.393460	-1.364382
C	1.801580	2.700188	-2.079291
C	2.812263	2.054473	-1.371913
C	3.282309	0.746567	-1.805664
C	3.562774	-0.043522	-0.615720
C	3.268339	-1.400274	-0.596952
C	2.663691	-2.002451	0.583971
C	1.716040	-3.001318	0.150201
C	0.516676	-3.153696	0.848362
C	-2.688180	-0.123693	1.645684
C	-1.774445	-2.721976	-2.019951
C	-2.793250	-2.055609	-1.343970
C	-3.257325	-0.761441	-1.822503
C	-2.681586	-0.189243	-2.954901
C	-1.617787	-0.886178	-3.660226
C	0.249103	-2.431898	-3.188880
C	0.529545	-3.218818	-1.999985
C	-0.720902	-3.394013	-1.272090
C	-0.725456	-3.354217	0.118333
C	-1.787094	-2.656538	0.826506
C	-2.807119	-2.029192	0.109093
C	-3.551501	0.064285	-0.660404
C	-3.259509	1.421692	-0.679072
C	-2.657675	2.021648	-1.859950
C	-2.375759	1.235280	-2.973924
C	-1.123044	1.415531	-3.691175

C	-0.654842	0.104839	-4.116640
C	0.706716	-0.188088	-4.104174
C	1.169574	-1.485052	-3.634303
C	1.718909	-3.023453	-1.302675
C	2.681183	-2.035188	-1.767002
C	2.413445	-1.283000	-2.907551
C	2.719549	0.141513	-2.927492
C	1.664365	0.816830	-3.665698
C	1.216760	2.069357	-3.249255
C	-0.208073	2.375578	-3.263576
C	-0.502755	3.197598	-2.101958
C	-1.700687	3.023193	-1.413646
C	-3.270324	-0.727869	0.529807
C	-2.669368	2.058316	0.490616
C	-1.175398	-2.125581	-3.200895
C	0.768694	-0.098391	3.165145
C	1.081526	-0.167686	4.689392
H	1.880479	-0.880385	4.914272
C	-0.802951	0.239753	3.149920
C	-1.144242	0.313870	4.667393
H	-1.021668	1.357856	5.018805
H	-2.170494	-0.003398	4.875024
N	-0.177085	-0.572600	5.283997
C	-0.178869	-0.516145	6.732055
H	-1.156198	-0.827192	7.113875
H	0.574466	-1.202744	7.130549
H	0.038007	0.500160	7.114209
H	1.395336	0.834548	5.043564

Geometry optimized structure of (*P*)-(12,8)-[4]CC⊃**1** with ωB97X/6-311G(d) (Fig. S1)

C	-6.924458	1.019243	-0.002517
C	-6.547430	1.787759	1.079012
C	-6.035371	3.097605	0.938798

C	-5.863307	3.633460	-0.354215
C	-6.447320	2.920129	-1.430845
C	-6.967954	1.664298	-1.262606
C	-5.544029	3.827993	2.082155
C	-4.962069	4.754233	-0.543335
C	-4.349745	5.332594	0.569434
C	-4.755521	4.912463	1.877609
C	-3.178844	6.165473	0.382223
C	-2.628451	6.302810	-0.908265
C	-3.388883	5.863676	-2.052596
C	-4.519871	5.140712	-1.849939
H	-6.508362	1.337413	2.064312
H	-6.443083	3.344462	-2.428983
H	-7.367514	1.142196	-2.126829
H	-4.354781	5.424711	2.746397
H	-5.052008	4.770853	-2.720599
C	-1.278247	6.704945	-1.040742
H	-0.824680	6.626367	-2.022630
C	-2.433215	6.699385	1.463088
H	-2.866600	6.737239	2.456560
C	-0.488672	7.007198	0.048328
C	-1.139059	7.114547	1.302971
H	-0.592843	7.478573	2.167950
C	0.996960	6.937065	-0.055128
C	1.746227	6.563190	1.040424
C	1.661644	6.974309	-1.304817
C	3.056737	6.046385	0.923420
H	1.278003	6.527246	2.017707
C	2.918948	6.450643	-1.450708
H	1.153290	7.370938	-2.178574
C	3.614447	5.870624	-0.360153
C	3.765187	5.554514	2.080058
H	3.359510	6.441920	-2.441738

C	4.744212	4.977074	-0.528065
C	4.852742	4.765288	1.895091
C	5.299972	4.363566	0.595118
C	5.165740	4.544375	-1.827099
H	5.347515	4.362864	2.773186
C	6.139246	3.195172	0.422028
C	5.896201	3.416652	-2.018267
H	4.817603	5.081479	-2.703625
C	6.307819	2.650090	-0.867328
C	6.653840	2.448684	1.511209
C	6.721550	1.302838	-0.995740
H	6.667947	2.878507	2.506821
C	7.080449	1.157681	1.355183
H	6.668211	0.853325	-1.981206
C	7.002958	0.510355	0.097163
H	7.428154	0.611228	2.226561
C	-6.996410	-0.464745	0.126976
C	-6.718121	-1.275901	-0.952970
C	-7.071312	-1.090385	1.396034
C	-6.304309	-2.620923	-0.802508
H	-6.667145	-0.843305	-1.946105
C	-6.644031	-2.378404	1.573141
H	-7.417390	-0.529125	2.258621
C	-6.131620	-3.143207	0.495686
C	-5.896292	-3.407834	-1.940945
H	-6.655974	-2.791432	2.575856
C	-5.290148	-4.307153	0.686930
C	-5.165203	-4.532043	-1.732042
C	-4.738566	-4.941039	-0.426973
C	-4.835351	-4.681884	1.992249
H	-4.819882	-5.084677	-2.600005
C	-3.607363	-5.830456	-0.247158
C	-3.745022	-5.464823	2.187265

H	-5.325225	-4.261727	2.864730
C	-3.042935	-5.979834	1.036859
C	-2.917091	-6.432040	-1.329402
C	-1.731691	-6.493803	1.157534
H	-3.362774	-6.443495	-2.318130
C	-1.658897	-6.952499	-1.179392
H	-1.258331	-6.437018	2.131331
C	-0.988173	-6.890237	0.066034
H	-1.154685	-7.366544	-2.047485
C	6.932025	-0.975672	-0.007204
C	6.558723	-1.726216	1.088127
C	6.972393	-1.641733	-1.256430
C	6.047252	-3.038564	0.971363
H	6.522362	-1.259657	2.065975
C	6.452159	-2.900571	-1.402060
H	7.369125	-1.134022	-2.130471
C	5.871649	-3.596103	-0.311988
C	5.559741	-3.749929	2.128207
H	6.445244	-3.341617	-2.392922
C	4.970336	-4.720252	-0.479690
C	4.771322	-4.838092	1.944174
C	4.361694	-5.280112	0.644439
C	4.523743	-5.128340	-1.778268
H	4.373310	-5.335746	2.822611
C	3.189796	-6.115443	0.475003
C	3.391879	-5.854249	-1.965081
H	5.053205	-4.773414	-2.656757
C	2.634763	-6.273664	-0.811112
C	2.447482	-6.630175	1.567268
C	1.283659	-6.676455	-0.932287
H	2.883906	-6.651363	2.559875
C	1.152374	-7.046482	1.418604
H	0.826505	-6.613824	-1.913729

C	0.497761	-6.959477	0.164652
H	0.608526	-7.394675	2.291523
C	-3.229464	-5.733278	3.575449
H	-2.288167	-5.204331	3.761597
H	-3.044229	-6.798733	3.740784
H	-3.946908	-5.396783	4.326415
C	-5.844355	3.347466	3.476269
H	-5.324309	2.408059	3.695084
H	-6.913775	3.169795	3.623094
H	-5.520790	4.081176	4.217163
C	-2.881953	6.122756	-3.445048
H	-1.990040	5.522107	-3.659287
H	-2.612444	7.172691	-3.591991
H	-3.637727	5.861844	-4.188348
C	3.259637	5.855135	3.465358
H	2.315557	5.337125	3.667896
H	3.081937	6.924966	3.609291
H	3.979315	5.529940	4.219180
C	6.194961	2.919744	-3.406606
H	5.606212	2.025710	-3.643146
H	7.250168	2.657708	-3.527172
H	5.949366	3.678849	-4.151733
C	5.863761	-3.245834	3.513182
H	5.345513	-2.302005	3.716972
H	6.933701	-3.066830	3.654600
H	5.541112	-3.966398	4.267272
C	2.880533	-6.136991	-3.351267
H	1.987843	-5.540133	-3.572694
H	2.610626	-7.189292	-3.479323
H	3.633877	-5.888774	-4.101365
C	-6.199511	-2.935794	-3.336990
H	-5.611306	-2.046350	-3.591565
H	-7.255044	-2.675645	-3.458854

H	-5.956523	-3.708235	-4.069161
C	1.243443	2.061485	1.969204
C	-0.201125	2.398728	1.970206
C	-1.124018	1.487838	2.401837
C	1.668742	0.836194	2.400924
C	1.826193	2.658863	0.793250
C	0.783861	3.358905	0.069319
C	-0.460146	3.193960	0.794586
C	-1.650032	3.051252	0.097785
C	-2.339488	1.309846	1.659486
C	-1.651141	-0.796241	2.404891
C	-1.232833	-2.024317	1.980462
C	0.210672	-2.361325	1.980295
C	1.129176	-1.444978	2.403475
C	2.345867	-1.272514	1.660687
C	2.679324	0.139505	1.657622
C	3.268674	0.710532	0.540176
C	2.830918	2.005938	0.096302
C	0.786898	3.374143	-1.311485
C	1.828626	2.674763	-2.040566
C	2.824404	2.007108	-1.352973
C	3.266656	0.702461	-1.804722
C	3.539765	-0.104058	-0.631233
C	3.224085	-1.445722	-0.627741
C	2.619460	-2.049213	0.546327
C	1.656518	-3.022052	0.108256
C	0.468044	-3.161369	0.807880
C	-2.666423	-0.103703	1.662963
C	-1.826103	-2.655738	-2.025322
C	-2.820275	-1.984582	-1.338635
C	-3.263323	-0.681910	-1.795436
C	-2.690434	-0.109753	-2.917700
C	-1.647980	-0.814012	-3.636809

C	0.186764	-2.387884	-3.200946
C	0.460482	-3.190770	-2.027049
C	-0.782988	-3.351967	-1.295109
C	-0.777273	-3.330051	0.085749
C	-1.817990	-2.626221	0.808313
C	-2.824176	-1.976875	0.110433
C	-3.533439	0.129965	-0.624698
C	-3.219696	1.472082	-0.628753
C	-2.618446	2.073937	-1.801980
C	-2.360535	1.303841	-2.921119
C	-1.114441	1.470806	-3.642233
C	-0.673992	0.162161	-4.086389
C	0.672763	-0.152036	-4.086930
C	1.114095	-1.458533	-3.637919
C	1.648817	-3.026099	-1.340522
C	2.621350	-2.053270	-1.797492
C	2.361495	-1.288179	-2.919564
C	2.691542	0.125364	-2.923347
C	1.647600	0.826299	-3.643356
C	1.227631	2.072046	-3.211004
C	-0.186285	2.402210	-3.211538
C	-0.457869	3.209692	-2.040437
C	-1.645060	3.048707	-1.351232
C	-3.259714	-0.679478	0.549891
C	-2.613403	2.080978	0.541451
C	-1.227100	-2.057707	-3.199227
C	0.785422	-0.156600	3.150810
C	1.111338	-0.249575	4.658883
H	1.897296	-0.980072	4.869596
C	-0.771326	0.206797	3.151457
C	-1.103005	0.268543	4.659877
H	-0.970520	1.305894	5.024278
H	-2.131236	-0.037102	4.871898

N	-0.145427	-0.631007	5.266632
C	-0.132483	-0.578598	6.710865
H	-1.108759	-0.874208	7.102887
H	0.611692	-1.276696	7.102070
H	0.103917	0.431119	7.094110
H	1.453514	0.738499	5.023644

Geometry optimized structure of (*P*)-(12,8)-[4]CC⊃**1** with ωB97/6-311G(d) (Fig. S1)

C	-6.924768	1.022930	-0.020851
C	-6.534146	1.784692	1.061623
C	-6.018645	3.095908	0.918749
C	-5.856361	3.632662	-0.375663
C	-6.451642	2.924087	-1.453507
C	-6.977411	1.669536	-1.283216
C	-5.513538	3.823121	2.062400
C	-4.951767	4.752349	-0.571354
C	-4.340399	5.338428	0.538357
C	-4.733435	4.914510	1.853691
C	-3.172601	6.178431	0.345534
C	-2.616654	6.299303	-0.944757
C	-3.366185	5.835996	-2.090768
C	-4.501771	5.119052	-1.885314
H	-6.485386	1.327876	2.046361
H	-6.455508	3.354397	-2.451402
H	-7.389324	1.148053	-2.144749
H	-4.323771	5.426063	2.721439
H	-5.026967	4.731400	-2.755110
C	-1.265234	6.705958	-1.076061
H	-0.801685	6.609851	-2.054458
C	-2.436412	6.732712	1.427211
H	-2.879347	6.783289	2.418300
C	-0.486090	7.030578	0.014914
C	-1.142598	7.153949	1.268369

H	-0.599318	7.534618	2.130899
C	1.000670	6.959747	-0.082611
C	1.741522	6.574016	1.015484
C	1.667882	7.001151	-1.334315
C	3.051959	6.049473	0.898231
H	1.265812	6.532570	1.991806
C	2.922539	6.468440	-1.479879
H	1.161534	7.408911	-2.206850
C	3.610584	5.877723	-0.386015
C	3.755139	5.545275	2.056991
H	3.369800	6.464059	-2.470259
C	4.736739	4.976863	-0.557163
C	4.846173	4.758871	1.870745
C	5.295889	4.363918	0.565106
C	5.139759	4.533331	-1.862744
H	5.338636	4.348507	2.749161
C	6.136198	3.193555	0.389732
C	5.860259	3.398086	-2.054224
H	4.778066	5.064146	-2.740242
C	6.289830	2.641527	-0.899180
C	6.663627	2.454155	1.482067
C	6.704764	1.292036	-1.024923
H	6.687645	2.892904	2.475964
C	7.092895	1.162124	1.328865
H	6.636503	0.832946	-2.007715
C	7.003462	0.509152	0.071178
H	7.452317	0.617928	2.199723
C	-6.997573	-0.462190	0.103929
C	-6.703009	-1.264187	-0.979410
C	-7.084533	-1.093161	1.372908
C	-6.288441	-2.611610	-0.831337
H	-6.637250	-0.822208	-1.970207
C	-6.655447	-2.382520	1.547371

H	-7.441575	-0.533575	2.234975
C	-6.130687	-3.140670	0.466667
C	-5.862219	-3.388601	-1.974008
H	-6.677272	-2.804291	2.548634
C	-5.287772	-4.306230	0.660418
C	-5.140687	-4.520024	-1.764456
C	-4.732439	-4.939383	-0.452481
C	-4.829892	-4.673329	1.971278
H	-4.781301	-5.066228	-2.633436
C	-3.603994	-5.834982	-0.269238
C	-3.735237	-5.452254	2.167504
H	-5.317705	-4.245569	2.843926
C	-3.038171	-5.979344	1.015265
C	-2.920909	-6.446996	-1.354539
C	-1.726632	-6.500126	1.136222
H	-3.373455	-6.463208	-2.342412
C	-1.664936	-6.975521	-1.204779
H	-1.245628	-6.437258	2.108790
C	-0.991499	-6.908245	0.042409
H	-1.162529	-7.400395	-2.071439
C	6.933067	-0.978039	-0.028377
C	6.548621	-1.722422	1.068282
C	6.981169	-1.645462	-1.280079
C	6.034228	-3.036434	0.949349
H	6.503779	-1.249657	2.045659
C	6.456376	-2.903346	-1.427252
H	7.388572	-1.137896	-2.151999
C	5.866565	-3.594627	-0.335286
C	5.534970	-3.745169	2.107041
H	6.456232	-3.350079	-2.417924
C	4.961782	-4.717870	-0.508556
C	4.754015	-4.839780	1.919734
C	4.354913	-5.285038	0.613310

C	4.506540	-5.107033	-1.814289
H	4.348374	-5.337111	2.797554
C	3.185151	-6.126519	0.439614
C	3.369863	-5.826929	-2.002905
H	5.028871	-4.735208	-2.692704
C	2.623754	-6.268826	-0.846156
C	2.452073	-6.659455	1.533874
C	1.270968	-6.674814	-0.965103
H	2.898295	-6.692801	2.524179
C	1.156661	-7.080224	1.387640
H	0.803698	-6.595870	-1.943318
C	0.495566	-6.978029	0.134778
H	0.615759	-7.443488	2.259079
C	-3.206914	-5.706262	3.556093
H	-2.262983	-5.173364	3.726315
H	-3.019015	-6.771429	3.730954
H	-3.919063	-5.360977	4.310603
C	-5.792827	3.328961	3.458539
H	-5.264798	2.388121	3.659142
H	-6.861031	3.145578	3.618928
H	-5.459985	4.058384	4.202097
C	-2.837990	6.061273	-3.483671
H	-1.945280	5.448923	-3.668729
H	-2.559626	7.107507	-3.651262
H	-3.585867	5.785928	-4.232262
C	3.237350	5.832453	3.443111
H	2.290217	5.310891	3.630155
H	3.057854	6.902397	3.596245
H	3.951692	5.498345	4.200604
C	6.126442	2.877341	-3.442936
H	5.522388	1.984116	-3.650546
H	7.177891	2.602730	-3.581848
H	5.870797	3.628595	-4.195130

C	5.821129	-3.228588	3.493654
H	5.295909	-2.283436	3.681104
H	6.890336	-3.044466	3.646406
H	5.490334	-3.945186	4.250489
C	2.836952	-6.077538	-3.389629
H	1.943732	-5.468477	-3.582807
H	2.557754	-7.126614	-3.536828
H	3.582375	-5.816301	-4.145706
C	-6.132425	-2.892596	-3.370975
H	-5.528920	-2.003221	-3.596124
H	-7.184258	-2.620440	-3.511851
H	-5.878843	-3.657077	-4.110441
C	1.232090	2.068236	2.028738
C	-0.217855	2.398119	2.028385
C	-1.136712	1.479342	2.457196
C	1.662935	0.842325	2.458721
C	1.815574	2.673428	0.853322
C	0.767131	3.371216	0.127878
C	-0.480809	3.197176	0.852419
C	-1.671773	3.049075	0.154091
C	-2.355021	1.296788	1.713823
C	-1.652083	-0.811069	2.456860
C	-1.227342	-2.038860	2.032275
C	0.221542	-2.368529	2.033296
C	1.134887	-1.445206	2.457945
C	2.356205	-1.266360	1.717412
C	2.682525	0.151068	1.716104
C	3.272741	0.728373	0.600104
C	2.826676	2.025371	0.156484
C	0.771475	3.387502	-1.254653
C	1.820255	2.691488	-1.984116
C	2.820939	2.027666	-1.296110
C	3.272016	0.722553	-1.749666

C	3.550007	-0.086326	-0.574523
C	3.240946	-1.431992	-0.572921
C	2.636606	-2.042655	0.602320
C	1.676783	-3.023047	0.161153
C	0.485633	-3.169627	0.859232
C	-2.674673	-0.122172	1.714975
C	-1.814135	-2.670424	-1.979542
C	-2.814832	-2.004772	-1.293148
C	-3.265666	-0.700536	-1.749662
C	-2.692416	-0.122753	-2.870770
C	-1.642503	-0.821956	-3.590289
C	0.203722	-2.388409	-3.154095
C	0.481336	-3.194562	-1.979333
C	-0.765693	-3.365057	-1.248137
C	-0.761914	-3.345483	0.134487
C	-1.810447	-2.645640	0.857797
C	-2.821298	-1.999423	0.159257
C	-3.543368	0.110871	-0.575933
C	-3.236361	1.457016	-0.577969
C	-2.634297	2.064956	-1.752048
C	-2.369577	1.295791	-2.872093
C	-1.120432	1.470553	-3.592366
C	-0.671291	0.162124	-4.038165
C	0.678468	-0.145002	-4.037501
C	1.127430	-1.452354	-3.588944
C	1.670137	-3.024266	-1.291074
C	2.640181	-2.042798	-1.746382
C	2.376178	-1.275938	-2.868114
C	2.699242	0.142555	-2.869885
C	1.649493	0.840176	-3.591024
C	1.221803	2.084460	-3.157535
C	-0.196894	2.407612	-3.159418
C	-0.475145	3.215481	-1.986128

C	-1.664448	3.047270	-1.298370
C	-3.266120	-0.701501	0.600564
C	-2.633155	2.070266	0.596293
C	-1.214911	-2.065220	-3.153532
C	0.781489	-0.157366	3.205840
C	1.106643	-0.251156	4.714820
H	1.900485	-0.975952	4.926308
C	-0.776051	0.197131	3.205122
C	-1.110635	0.254629	4.713870
H	-0.978024	1.292373	5.082801
H	-2.140416	-0.053881	4.924963
N	-0.149957	-0.645729	5.319790
C	-0.136382	-0.583614	6.765896
H	-1.112534	-0.881973	7.161189
H	0.613533	-1.275684	7.161893
H	0.095170	0.432218	7.140227
H	1.437179	0.741255	5.084221

Geometry optimized structure of (*P*)-(12,8)-[4]CC⊃**1** with M06-2X/6-311G(d) (Fig. S1)

C	-6.916035	1.011049	-0.030832
C	-6.501220	1.757978	1.053528
C	-5.980080	3.061229	0.911079
C	-5.829804	3.601232	-0.386823
C	-6.450002	2.911171	-1.457267
C	-6.987258	1.663190	-1.285612
C	-5.459691	3.776971	2.046518
C	-4.921422	4.705742	-0.588921
C	-4.308586	5.299139	0.521488
C	-4.685118	4.872860	1.833619
C	-3.158155	6.147698	0.321736
C	-2.596369	6.250468	-0.971079
C	-3.330534	5.765867	-2.109387

C	-4.468938	5.052963	-1.899910
H	-6.438271	1.290639	2.028169
H	-6.472268	3.351003	-2.446162
H	-7.425988	1.153205	-2.135731
H	-4.261603	5.373289	2.695963
H	-4.980465	4.646172	-2.763785
C	-1.251820	6.660069	-1.100016
H	-0.776931	6.542842	-2.066251
C	-2.441956	6.735637	1.393829
H	-2.896403	6.810935	2.373584
C	-0.487922	7.014305	-0.007129
C	-1.152197	7.166370	1.235065
H	-0.619248	7.577626	2.085030
C	0.987682	6.942844	-0.094705
C	1.713254	6.533905	1.005447
C	1.660629	7.002739	-1.338723
C	3.015157	6.002473	0.889030
H	1.226574	6.478587	1.971266
C	2.908471	6.457951	-1.485245
H	1.165615	7.436746	-2.200133
C	3.577250	5.841749	-0.398606
C	3.705939	5.483885	2.040180
H	3.365213	6.471471	-2.466534
C	4.691507	4.940754	-0.574704
C	4.803913	4.705910	1.851296
C	5.258441	4.328704	0.549539
C	5.081103	4.497873	-1.877222
H	5.284395	4.281828	2.724635
C	6.109101	3.176644	0.369007
C	5.799152	3.360731	-2.071512
H	4.703500	5.016241	-2.750198
C	6.246489	2.618478	-0.922571
C	6.671986	2.459525	1.453238

C	6.668914	1.277279	-1.045248
H	6.720286	2.910784	2.436109
C	7.113736	1.172497	1.301176
H	6.581469	0.806176	-2.016478
C	6.996940	0.510754	0.054415
H	7.505015	0.639871	2.160589
C	-6.989771	-0.463092	0.083821
C	-6.665082	-1.249822	-1.002547
C	-7.103541	-1.101858	1.342706
C	-6.243192	-2.588865	-0.856662
H	-6.580333	-0.796845	-1.982582
C	-6.661820	-2.386106	1.517006
H	-7.492463	-0.553581	2.193304
C	-6.102098	-3.123122	0.444548
C	-5.799733	-3.352485	-1.993032
H	-6.707627	-2.819585	2.507974
C	-5.250237	-4.271152	0.643859
C	-5.082180	-4.486587	-1.779875
C	-4.688125	-4.905074	-0.470609
C	-4.788292	-4.620478	1.950756
H	-4.707522	-5.021301	-2.644225
C	-3.572682	-5.802046	-0.281751
C	-3.687880	-5.392414	2.149972
H	-5.263646	-4.177720	2.817595
C	-3.003558	-5.934977	1.005978
C	-2.908908	-6.439988	-1.358945
C	-1.700442	-6.462326	1.126394
H	-3.370937	-6.474250	-2.337268
C	-1.659570	-6.980202	-1.207885
H	-1.208466	-6.385222	2.088034
C	-0.980506	-6.893935	0.031164
H	-1.168216	-7.431089	-2.062739
C	6.923357	-0.965210	-0.033091

C	6.508354	-1.691167	1.065305
C	6.994228	-1.640965	-1.275308
C	5.987478	-2.996946	0.947950
H	6.445228	-1.205116	2.030742
C	6.456889	-2.892077	-1.422982
H	7.432702	-1.147101	-2.135057
C	5.837043	-3.561717	-0.339437
C	5.467399	-3.690574	2.097066
H	6.478803	-3.350791	-2.403291
C	4.928666	-4.670052	-0.520004
C	4.694476	-4.791506	1.905583
C	4.317888	-5.243186	0.602028
C	4.473619	-5.041321	-1.823571
H	4.270817	-5.274978	2.777434
C	3.167133	-6.095273	0.419992
C	3.334546	-5.757675	-2.017743
H	4.983791	-4.650880	-2.695793
C	2.601905	-6.220605	-0.869347
C	2.453625	-6.663258	1.504359
C	1.256283	-6.630463	-0.987408
H	2.910574	-6.721658	2.484070
C	1.163015	-7.095078	1.356843
H	0.778584	-6.530404	-1.954283
C	0.495330	-6.963962	0.114160
H	0.631843	-7.490313	2.215436
C	-3.140893	-5.611921	3.534086
H	-2.202727	-5.066106	3.677534
H	-2.939504	-6.668685	3.725682
H	-3.845955	-5.258782	4.286646
C	-5.707986	3.268091	3.440161
H	-5.166793	2.333298	3.619128
H	-6.768557	3.071677	3.615081
H	-5.370096	3.993150	4.180678

C	-2.786425	5.954604	-3.498398
H	-1.897345	5.333959	-3.656238
H	-2.500338	6.992528	-3.684496
H	-3.526552	5.666168	-4.244826
C	3.169004	5.736733	3.422567
H	2.227615	5.201267	3.583082
H	2.975448	6.798696	3.592308
H	3.876337	5.395430	4.178480
C	6.035284	2.826197	-3.457222
H	5.421631	1.937747	-3.642252
H	7.079373	2.542738	-3.610008
H	5.771420	3.571364	-4.207716
C	5.712927	-3.153006	3.480416
H	5.171692	-2.214348	3.638397
H	6.773107	-2.953073	3.653782
H	5.373136	-3.862499	4.235020
C	2.788254	-5.972771	-3.402048
H	1.899727	-5.354165	-3.570623
H	2.500566	-7.013781	-3.567217
H	3.527692	-5.700015	-4.155040
C	-6.038772	-2.842960	-3.387618
H	-5.425230	-1.958156	-3.589844
H	-7.083086	-2.561921	-3.543386
H	-5.776627	-3.601534	-4.125171
C	1.255839	2.059312	2.053960
C	-0.186872	2.401585	2.057117
C	-1.114698	1.490135	2.486449
C	1.677766	0.828303	2.482388
C	1.843296	2.660802	0.880818
C	0.800880	3.367095	0.160109
C	-0.445502	3.204951	0.885276
C	-1.642107	3.066833	0.189008
C	-2.333956	1.317903	1.747875

C	-1.650317	-0.793035	2.487241
C	-1.237013	-2.025939	2.062716
C	0.204620	-2.368123	2.060789
C	1.128448	-1.451684	2.481173
C	2.347705	-1.283340	1.740624
C	2.686677	0.128292	1.738999
C	3.284833	0.701879	0.622635
C	2.850102	2.002547	0.181326
C	0.802495	3.383875	-1.224767
C	1.841431	2.678147	-1.954022
C	2.840577	2.004147	-1.267673
C	3.276888	0.695898	-1.721022
C	3.550952	-0.114786	-0.549529
C	3.228604	-1.460683	-0.547476
C	2.621901	-2.065477	0.625686
C	1.652688	-3.036420	0.188144
C	0.459070	-3.173291	0.889558
C	-2.665925	-0.095369	1.749706
C	-1.839383	-2.652143	-1.941595
C	-2.835529	-1.976549	-1.252327
C	-3.273634	-0.669116	-1.706455
C	-2.694824	-0.094893	-2.828772
C	-1.654938	-0.802133	-3.548385
C	0.175459	-2.386668	-3.116230
C	0.447756	-3.195386	-1.946286
C	-0.797590	-3.356797	-1.215220
C	-0.790266	-3.337172	0.169753
C	-1.829416	-2.628665	0.893061
C	-2.839322	-1.972283	0.196517
C	-3.542190	0.143828	-0.534976
C	-3.221753	1.490181	-0.537752
C	-2.616366	2.091684	-1.710278
C	-2.359840	1.318239	-2.831204

C	-1.112430	1.480732	-3.551189
C	-0.677506	0.171019	-3.996386
C	0.671240	-0.148784	-3.998753
C	1.108007	-1.457464	-3.553032
C	1.642566	-3.036393	-1.260381
C	2.619195	-2.064836	-1.716798
C	2.358274	-1.293453	-2.838052
C	2.693396	0.119628	-2.839889
C	1.650500	0.825415	-3.556344
C	1.235286	2.075951	-3.121841
C	-0.178052	2.410860	-3.120344
C	-0.445732	3.221087	-1.950560
C	-1.637929	3.064028	-1.259798
C	-3.270676	-0.670764	0.637668
C	-2.610948	2.097390	0.631851
C	-1.237795	-2.051698	-3.112643
C	0.790490	-0.162618	3.227672
C	1.115716	-0.263871	4.737593
H	1.902717	-0.992537	4.942225
C	-0.765439	0.206560	3.230544
C	-1.095124	0.263233	4.741766
H	-0.942293	1.293869	5.111247
H	-2.125383	-0.031416	4.950849
N	-0.145285	-0.657700	5.335056
C	-0.132560	-0.615728	6.783199
H	-1.109865	-0.910407	7.168811
H	0.608728	-1.319211	7.165625
H	0.107257	0.389595	7.169551
H	1.446500	0.723931	5.107640

Geometry optimized structure of (*P*)-(12,8)-[4]CC⊃**1** with B97-D/6-311G(d) (Fig. S1)

C	-7.016229	1.030590	-0.064217
C	-6.594781	1.785897	1.030343

C	-6.032780	3.075813	0.887712
C	-5.858557	3.613268	-0.429581
C	-6.505328	2.934109	-1.499850
C	-7.074893	1.689129	-1.325434
C	-5.494450	3.782134	2.023215
C	-4.919686	4.694728	-0.632266
C	-4.296868	5.294145	0.496817
C	-4.689442	4.873044	1.806898
C	-3.146336	6.147410	0.298087
C	-2.573050	6.253719	-1.011357
C	-3.296867	5.749446	-2.150411
C	-4.448078	5.030262	-1.940095
H	-6.550883	1.319712	2.010978
H	-6.518034	3.373198	-2.495248
H	-7.518091	1.181046	-2.181269
H	-4.250799	5.356981	2.677425
H	-4.942899	4.606559	-2.811585
C	-1.235496	6.696204	-1.137225
H	-0.755305	6.591368	-2.106153
C	-2.436088	6.755630	1.370859
H	-2.893177	6.827745	2.355726
C	-0.466618	7.062193	-0.033044
C	-1.141038	7.206012	1.213199
H	-0.609433	7.618199	2.070477
C	1.006499	6.990634	-0.120041
C	1.737070	6.565288	0.989385
C	1.690479	7.054329	-1.366536
C	3.034250	6.012911	0.874291
H	1.246605	6.514423	1.957888
C	2.943179	6.493812	-1.514768
H	1.196900	7.495115	-2.232088
C	3.605342	5.852027	-0.430896
C	3.717092	5.474242	2.023836

H	3.403044	6.511821	-2.500568
C	4.706099	4.931681	-0.612154
C	4.822159	4.683190	1.829439
C	5.281069	4.306117	0.527776
C	5.088424	4.478881	-1.914358
H	5.287608	4.241455	2.708494
C	6.148891	3.164452	0.342519
C	5.820473	3.334533	-2.114377
H	4.691744	4.982319	-2.793622
C	6.291985	2.600658	-0.967402
C	6.741791	2.454658	1.424003
C	6.746042	1.266381	-1.090151
H	6.790045	2.907992	2.412101
C	7.209605	1.165555	1.268676
H	6.665987	0.792157	-2.064399
C	7.093671	0.493936	0.017952
H	7.611661	0.635951	2.131876
C	-7.086719	-0.441078	0.053527
C	-6.742799	-1.235326	-1.040327
C	-7.197927	-1.087742	1.317758
C	-6.286911	-2.566485	-0.892484
H	-6.667315	-0.780758	-2.024287
C	-6.727396	-2.372666	1.497228
H	-7.598323	-0.541725	2.171450
C	-6.137053	-3.102767	0.428065
C	-5.820065	-3.323930	-2.025968
H	-6.771823	-2.806820	2.494099
C	-5.265103	-4.237758	0.633267
C	-5.086647	-4.463724	-1.805445
C	-4.696683	-4.888161	-0.495959
C	-4.794730	-4.581217	1.939982
H	-4.693866	-4.985277	-2.675852
C	-3.594324	-5.803748	-0.300914

C	-3.686355	-5.364871	2.145008
H	-5.252285	-4.116564	2.811318
C	-3.013787	-5.933094	1.003652
C	-2.939863	-6.471028	-1.374093
C	-1.716568	-6.484340	1.122696
H	-3.406656	-6.511454	-2.355987
C	-1.686625	-7.029230	-1.221437
H	-1.218772	-6.409860	2.085888
C	-0.994693	-6.937795	0.018831
H	-1.198813	-7.490196	-2.079754
C	7.023189	-0.979754	-0.070989
C	6.605117	-1.713925	1.039104
C	7.079049	-1.662535	-1.319368
C	6.044218	-3.007004	0.923002
H	6.563515	-1.228761	2.010612
C	6.509931	-2.911054	-1.468182
H	7.519851	-1.170932	-2.185995
C	5.866811	-3.569987	-0.383201
C	5.510363	-3.692175	2.073404
H	6.520342	-3.369395	-2.454897
C	4.928629	-4.656244	-0.562273
C	4.706944	-4.788645	1.880575
C	4.310819	-5.235260	0.580063
C	4.452292	-5.016471	-1.861804
H	4.271688	-5.256334	2.761590
C	3.160109	-6.092812	0.401718
C	3.300602	-5.740051	-2.054214
H	4.943507	-4.608877	-2.742976
C	2.581116	-6.222785	-0.903104
C	2.454615	-6.681042	1.488543
C	1.242529	-6.666084	-1.015037
H	2.915913	-6.735586	2.472547
C	1.158471	-7.132771	1.344907

H	0.757621	-6.578631	-1.983398
C	0.478621	-7.010636	0.099414
H	0.629891	-7.528100	2.211923
C	-3.128849	-5.550215	3.536861
H	-2.169504	-5.020737	3.651998
H	-2.941952	-6.610584	3.762772
H	-3.821262	-5.153499	4.290074
C	-5.737247	3.278387	3.426696
H	-5.231102	2.313720	3.593231
H	-6.807970	3.117729	3.621803
H	-5.353824	3.990213	4.168652
C	-2.743222	5.911516	-3.545535
H	-1.825604	5.314968	-3.673311
H	-2.481644	6.957924	-3.761548
H	-3.468881	5.573653	-4.295923
C	3.174647	5.700743	3.415583
H	2.211606	5.183429	3.553722
H	2.998320	6.768265	3.614811
H	3.871131	5.318589	4.172592
C	6.036052	2.799541	-3.509994
H	5.452053	1.879424	-3.671838
H	7.091671	2.548894	-3.691567
H	5.719816	3.532736	-4.262547
C	5.756026	-3.160922	3.466239
H	5.250229	-2.193119	3.614886
H	6.827098	-2.996148	3.655940
H	5.374472	-3.858305	4.222765
C	2.741787	-5.928938	-3.443762
H	1.823635	-5.334836	-3.579059
H	2.479460	-6.979302	-3.638570
H	3.464492	-5.605461	-4.203303
C	-6.041930	-2.818042	-3.431366
H	-5.458922	-1.901292	-3.614658

H	-7.098392	-2.571448	-3.613599
H	-5.728625	-3.566514	-4.169975
C	1.196959	2.088239	2.124783
C	-0.251075	2.394757	2.124563
C	-1.172110	1.455194	2.555404
C	1.658110	0.856340	2.557252
C	1.777165	2.712041	0.952454
C	0.718538	3.396489	0.230431
C	-0.527732	3.200396	0.951507
C	-1.730913	3.034343	0.243407
C	-2.383458	1.252541	1.806649
C	-1.653889	-0.850136	2.543569
C	-1.198826	-2.080889	2.108893
C	0.248307	-2.387320	2.109842
C	1.162573	-1.446036	2.543766
C	2.378541	-1.241259	1.803087
C	2.683575	0.180395	1.808848
C	3.276027	0.778341	0.683811
C	2.811453	2.074127	0.245531
C	0.723627	3.418254	-1.169225
C	1.783830	2.740561	-1.899209
C	2.808883	2.081931	-1.204472
C	3.278267	0.783132	-1.661984
C	3.568584	-0.027203	-0.491211
C	3.276577	-1.396234	-0.495441
C	2.679572	-2.020184	0.674065
C	1.732559	-3.014918	0.228235
C	0.527874	-3.185163	0.932658
C	-2.681666	-0.170599	1.801454
C	-1.777867	-2.708564	-1.919868
C	-2.804114	-2.053713	-1.222967
C	-3.272412	-0.751977	-1.673617
C	-2.700116	-0.152740	-2.804877

C	-1.638428	-0.833253	-3.526747
C	0.238247	-2.390538	-3.090130
C	0.526672	-3.197241	-1.919368
C	-0.719137	-3.391116	-1.191915
C	-0.716825	-3.377298	0.208023
C	-1.776593	-2.696469	0.931667
C	-2.809724	-2.054690	0.226849
C	-3.564556	0.051223	-0.498014
C	-3.274216	1.420627	-0.493930
C	-2.679120	2.042954	-1.664121
C	-2.398463	1.272130	-2.800238
C	-1.150436	1.468294	-3.518499
C	-0.681185	0.167895	-3.968466
C	0.691561	-0.122760	-3.967900
C	1.159904	-1.425678	-3.525217
C	1.728908	-3.011752	-1.221348
C	2.684566	-2.011699	-1.671075
C	2.406457	-1.233796	-2.802866
C	2.708330	0.191034	-2.798263
C	1.647966	0.875882	-3.517801
C	1.195992	2.128984	-3.075107
C	-0.229608	2.430576	-3.076103
C	-0.520474	3.228939	-1.900456
C	-1.724223	3.039881	-1.206415
C	-3.273852	-0.761638	0.672486
C	-2.680259	2.037601	0.680840
C	-1.187253	-2.088904	-3.090167
C	0.789499	-0.164043	3.294572
C	1.111272	-0.260179	4.815594
H	1.915562	-0.976972	5.025941
C	-0.792865	0.171031	3.294057
C	-1.126303	0.215493	4.814914
H	-1.006786	1.258294	5.186206

H	-2.152734	-0.111673	5.025209
N	-0.148136	-0.683037	5.414842
C	-0.138460	-0.635626	6.870244
H	-1.116673	-0.953147	7.255914
H	0.625897	-1.323449	7.256396
H	0.078321	0.384924	7.256950
H	1.426514	0.740764	5.187515

Geometry optimized structure of (*P*)-(12,8)-[4]CC⊃**1** with ωB97X-D/6-311G(d) (Fig. S1)

C	-6.930122	1.021715	-0.032761
C	-6.503247	1.762765	1.048333
C	-5.977126	3.062889	0.910259
C	-5.836098	3.608277	-0.384260
C	-6.468427	2.925755	-1.450034
C	-7.009248	1.680153	-1.280993
C	-5.441843	3.768458	2.043460
C	-4.924221	4.709269	-0.589020
C	-4.304052	5.296260	0.516993
C	-4.670122	4.863648	1.827915
C	-3.152125	6.141540	0.313108
C	-2.593875	6.242101	-0.979196
C	-3.332734	5.758797	-2.113655
C	-4.473709	5.054800	-1.899057
H	-6.433152	1.290186	2.019820
H	-6.495925	3.368265	-2.438303
H	-7.453518	1.177312	-2.133239
H	-4.235006	5.357522	2.688781
H	-4.990650	4.649730	-2.760981
C	-1.250903	6.652008	-1.109788
H	-0.778888	6.534673	-2.077076
C	-2.432176	6.728929	1.380393
H	-2.881792	6.804695	2.363082

C	-0.482646	7.005899	-0.022267
C	-1.143749	7.158569	1.218828
H	-0.611019	7.567884	2.070550
C	0.993791	6.930705	-0.113526
C	1.719381	6.519302	0.983482
C	1.667642	6.989381	-1.354219
C	3.020165	5.988370	0.870537
H	1.232738	6.463695	1.949048
C	2.915160	6.445727	-1.498572
H	1.175289	7.419458	-2.219776
C	3.584651	5.831043	-0.414176
C	3.707936	5.467505	2.021018
H	3.370014	6.457872	-2.481473
C	4.698619	4.929612	-0.590013
C	4.807085	4.694634	1.831472
C	5.264457	4.319195	0.532143
C	5.084579	4.481549	-1.889734
H	5.286617	4.268647	2.704919
C	6.117556	3.168946	0.352540
C	5.800398	3.344857	-2.084026
H	4.703571	4.997355	-2.763187
C	6.253772	2.607958	-0.935579
C	6.685139	2.456549	1.435150
C	6.680337	1.268882	-1.052984
H	6.734087	2.908604	2.418328
C	7.130411	1.171693	1.286948
H	6.591890	0.794375	-2.022171
C	7.012909	0.505673	0.045148
H	7.523074	0.645168	2.150225
C	-7.004464	-0.453696	0.080170
C	-6.675723	-1.238915	-1.003614
C	-7.119308	-1.094730	1.335235
C	-6.250030	-2.575903	-0.860786

H	-6.589704	-0.783873	-1.982281
C	-6.674159	-2.376571	1.507779
H	-7.509844	-0.551071	2.188802
C	-6.109719	-3.110471	0.438024
C	-5.800948	-3.336773	-1.995255
H	-6.720614	-2.809483	2.499677
C	-5.254435	-4.255528	0.638633
C	-5.085528	-4.469978	-1.779855
C	-4.694058	-4.890535	-0.472548
C	-4.787870	-4.598440	1.943577
H	-4.707872	-5.004109	-2.643717
C	-3.578539	-5.787126	-0.282316
C	-3.685509	-5.363829	2.144529
H	-5.261225	-4.150716	2.809467
C	-3.005878	-5.912867	1.002310
C	-2.914737	-6.426444	-1.356040
C	-1.703836	-6.439446	1.119718
H	-3.375496	-6.462300	-2.335612
C	-1.665519	-6.964868	-1.206616
H	-1.211148	-6.359150	2.080448
C	-0.984670	-6.876333	0.028375
H	-1.177112	-7.413961	-2.064770
C	6.939847	-0.971725	-0.038763
C	6.517844	-1.691879	1.058199
C	7.014176	-1.654086	-1.274365
C	5.991869	-2.994605	0.947458
H	6.451447	-1.200856	2.020737
C	6.473511	-2.903093	-1.417020
H	7.454176	-1.167341	-2.138109
C	5.845963	-3.565257	-0.335672
C	5.461346	-3.677862	2.096365
H	6.496660	-3.364536	-2.396735
C	4.933913	-4.670584	-0.515202

C	4.688657	-4.776812	1.905308
C	4.317441	-5.234847	0.604557
C	4.479452	-5.043859	-1.816366
H	4.256693	-5.253474	2.777347
C	3.163697	-6.082565	0.422037
C	3.337641	-5.751944	-2.012640
H	4.994933	-4.659023	-2.688384
C	2.600587	-6.208757	-0.865952
C	2.447012	-6.646645	1.503722
C	1.256354	-6.618655	-0.983478
H	2.899558	-6.703103	2.486289
C	1.157485	-7.077598	1.355585
H	0.780807	-6.521106	-1.951340
C	0.492044	-6.949402	0.114202
H	0.627157	-7.468322	2.217437
C	-3.133127	-5.565015	3.528558
H	-2.195429	-5.014859	3.663933
H	-2.928818	-6.619013	3.737105
H	-3.834584	-5.203640	4.282358
C	-5.665719	3.249894	3.436920
H	-5.123507	2.311792	3.600095
H	-6.723574	3.055357	3.634890
H	-5.311092	3.966395	4.179733
C	-2.793754	5.939358	-3.504943
H	-1.904403	5.318575	-3.663504
H	-2.509548	6.976740	-3.702198
H	-3.534170	5.645180	-4.250505
C	3.167583	5.707351	3.403642
H	2.226751	5.167921	3.559485
H	2.971507	6.767630	3.586666
H	3.872313	5.360655	4.161298
C	6.028367	2.808352	-3.469527
H	5.419635	1.914813	-3.648750

H	7.073626	2.532154	-3.634032
H	5.752696	3.547685	-4.223223
C	5.690706	-3.132247	3.478591
H	5.150591	-2.190162	3.625212
H	6.749473	-2.935274	3.669162
H	5.337772	-3.833679	4.236468
C	2.796359	-5.965677	-3.398255
H	1.906794	-5.348865	-3.570390
H	2.511658	-7.007520	-3.569596
H	3.535638	-5.689888	-4.151954
C	-6.032051	-2.828410	-3.390807
H	-5.422120	-1.939834	-3.589894
H	-7.077243	-2.553676	-3.558171
H	-5.759731	-3.583495	-4.129965
C	1.225382	2.055125	2.074677
C	-0.217864	2.382428	2.076328
C	-1.136269	1.461744	2.499129
C	1.658522	0.828765	2.497720
C	1.805964	2.663951	0.906344
C	0.761529	3.361642	0.188233
C	-0.480783	3.184136	0.908731
C	-1.670665	3.037031	0.209829
C	-2.347930	1.280461	1.757274
C	-1.648096	-0.822509	2.487153
C	-1.221142	-2.046503	2.057657
C	0.221045	-2.373709	2.057376
C	1.133934	-1.452636	2.484653
C	2.348483	-1.267657	1.747650
C	2.672819	0.143960	1.754139
C	3.263173	0.726801	0.642195
C	2.817548	2.020885	0.206980
C	0.765940	3.385264	-1.193263
C	1.811215	2.696939	-1.922647

C	2.811376	2.029816	-1.238238
C	3.261638	0.732688	-1.696182
C	3.540032	-0.078459	-0.530776
C	3.232103	-1.423924	-0.536056
C	2.630045	-2.037822	0.630108
C	1.674976	-3.013255	0.186611
C	0.484949	-3.165761	0.883859
C	-2.665563	-0.132711	1.751715
C	-1.806215	-2.656831	-1.944528
C	-2.806478	-1.994771	-1.255065
C	-3.256602	-0.693998	-1.703029
C	-2.685123	-0.110228	-2.820896
C	-1.638718	-0.802308	-3.540834
C	0.203486	-2.367899	-3.112667
C	0.480525	-3.175903	-1.946919
C	-0.761202	-3.351356	-1.220169
C	-0.757011	-3.337773	0.161551
C	-1.801399	-2.645064	0.884439
C	-2.813007	-1.997072	0.190083
C	-3.534350	0.108052	-0.530933
C	-3.228278	1.453914	-0.526354
C	-2.629347	2.065992	-1.691865
C	-2.364946	1.303371	-2.815508
C	-1.120557	1.482021	-3.531585
C	-0.672048	0.181148	-3.981469
C	0.677920	-0.124607	-3.982367
C	1.126278	-1.428804	-3.542701
C	1.668500	-3.007111	-1.258247
C	2.634392	-2.027301	-1.706985
C	2.370357	-1.255661	-2.824490
C	2.690758	0.157906	-2.818942
C	1.644478	0.855561	-3.533526
C	1.216087	2.097558	-3.094276

C	-0.197820	2.417783	-3.094265
C	-0.475326	3.215557	-1.921836
C	-1.663666	3.042085	-1.235261
C	-3.257356	-0.706529	0.635794
C	-2.627364	2.058860	0.644952
C	-1.210327	-2.047578	-3.110623
C	0.782083	-0.173202	3.237391
C	1.106586	-0.274778	4.745457
H	1.895357	-1.002457	4.949736
C	-0.777073	0.180210	3.238431
C	-1.111052	0.229805	4.746978
H	-0.987300	1.265918	5.116357
H	-2.136713	-0.084501	4.953176
N	-0.148919	-0.668913	5.345708
C	-0.142061	-0.643319	6.790323
H	-1.118027	-0.952850	7.170818
H	0.604760	-1.344391	7.169597
H	0.086194	0.359693	7.195228
H	1.444271	0.712350	5.115338

Global minimum of (*P*)-(12,8)-[4]CC⊃**1**+ for idealized rolling motions with LC-BLYP/6-311G(d) (Fig. S3)

C	-6.875348	1.010958	0.012169
C	-6.521517	1.781192	1.084373
C	-6.009683	3.080746	0.943575
C	-5.820190	3.604041	-0.336993
C	-6.387967	2.890483	-1.409736
C	-6.904161	1.645831	-1.243237
C	-5.542172	3.817384	2.082116
C	-4.924303	4.718318	-0.519038
C	-4.321139	5.287266	0.586227
C	-4.746029	4.881576	1.883957
C	-3.153311	6.109491	0.406312

C	-2.613402	6.261188	-0.871839
C	-3.376626	5.844722	-2.011915
C	-4.491025	5.117651	-1.815393
H	-6.507620	1.343347	2.072543
H	-6.376143	3.311848	-2.406003
H	-7.296526	1.122631	-2.106513
H	-4.370021	5.409261	2.750988
H	-5.034015	4.769903	-2.684653
C	-1.273587	6.664334	-1.006291
H	-0.831811	6.609596	-1.991575
C	-2.406886	6.627176	1.482548
H	-2.838300	6.660868	2.474105
C	-0.484013	6.948374	0.071492
C	-1.124561	7.039286	1.322548
H	-0.577741	7.400224	2.184977
C	0.992941	6.881663	-0.038973
C	1.746428	6.530475	1.045514
C	1.645549	6.906130	-1.285019
C	3.047600	6.017048	0.925380
H	1.292368	6.518038	2.026511
C	2.892557	6.389409	-1.431765
H	1.134272	7.295755	-2.156698
C	3.591406	5.826430	-0.346697
C	3.765102	5.550466	2.076354
H	3.328645	6.374951	-2.421662
C	4.715115	4.939292	-0.509694
C	4.834274	4.756779	1.895676
C	5.265122	4.336588	0.604969
C	5.146134	4.514246	-1.798776
H	5.346995	4.380520	2.771548
C	6.094177	3.171911	0.437923
C	5.879795	3.402718	-1.984460
H	4.816900	5.060915	-2.672938

C	6.272373	2.635113	-0.838405
C	6.597290	2.427059	1.521812
C	6.685042	1.297398	-0.967146
H	6.611962	2.857823	2.514090
C	7.019505	1.147282	1.367304
H	6.650913	0.857456	-1.954239
C	6.952318	0.507234	0.114973
H	7.368317	0.602166	2.235678
C	-6.942903	-0.464563	0.144664
C	-6.678386	-1.272089	-0.925191
C	-7.007507	-1.084830	1.407139
C	-6.265351	-2.607524	-0.776080
H	-6.646779	-0.847870	-1.919190
C	-6.584983	-2.362049	1.581102
H	-7.355066	-0.525786	2.267132
C	-6.084295	-3.124163	0.508094
C	-5.875970	-3.393309	-1.910859
H	-6.598753	-2.777431	2.580017
C	-5.255049	-4.286255	0.691055
C	-5.142366	-4.502191	-1.709768
C	-4.708161	-4.906844	-0.415279
C	-4.820882	-4.686852	1.986936
H	-4.815707	-5.062611	-2.576110
C	-3.584354	-5.791855	-0.241438
C	-3.751770	-5.478434	2.176891
H	-5.332644	-4.297925	2.857931
C	-3.036950	-5.963162	1.031812
C	-2.888936	-6.371977	-1.319583
C	-1.735630	-6.475202	1.156062
H	-3.327901	-6.372701	-2.308272
C	-1.641606	-6.886583	-1.168577
H	-1.278282	-6.448981	2.135315
C	-0.985138	-6.842684	0.074855

H	-1.132955	-7.289691	-2.035618
C	6.883529	-0.970210	0.006495
C	6.533008	-1.723173	1.092060
C	6.908777	-1.625512	-1.238449
C	6.020359	-3.024568	0.973498
H	6.522643	-1.269242	2.072963
C	6.391701	-2.872480	-1.383557
H	7.298748	-1.116293	-2.111093
C	5.826915	-3.568404	-0.297822
C	5.556849	-3.743483	2.125076
H	6.376990	-3.309714	-2.372922
C	4.929814	-4.684954	-0.459137
C	4.760419	-4.810964	1.946616
C	4.330768	-5.236945	0.656897
C	4.491539	-5.103657	-1.747619
H	4.388963	-5.326271	2.823111
C	3.162406	-6.061784	0.493683
C	3.376249	-5.833242	-1.929135
H	5.031114	-4.768727	-2.623973
C	2.617670	-6.232621	-0.779986
C	2.420399	-6.564653	1.580102
C	1.277425	-6.637941	-0.903253
H	2.856993	-6.585673	2.569817
C	1.137676	-6.979835	1.431123
H	0.831889	-6.597250	-1.887511
C	0.492162	-6.907156	0.181357
H	0.594703	-7.330761	2.300200
C	-3.279469	-5.815281	3.554843
H	-2.325145	-5.333809	3.784334
H	-3.133250	-6.889258	3.678716
H	-4.002470	-5.490840	4.301916
C	-5.898936	3.370693	3.463359
H	-5.416252	2.423648	3.718276

H	-6.974184	3.222693	3.573428
H	-5.588005	4.108532	4.201447
C	-2.895035	6.154471	-3.391841
H	-1.997379	5.582322	-3.639995
H	-2.648511	7.210934	-3.505916
H	-3.653609	5.907588	-4.132648
C	3.294432	5.905708	3.450107
H	2.344648	5.421097	3.690136
H	3.142825	6.980677	3.557904
H	4.020815	5.596242	4.200090
C	6.223529	2.928573	-3.359176
H	5.661803	2.029615	-3.625390
H	7.283599	2.687721	-3.449890
H	5.990393	3.689643	-4.101871
C	5.919843	-3.275617	3.497697
H	5.441411	-2.322870	3.739253
H	6.995799	-3.128248	3.601148
H	5.610929	-4.001386	4.248650
C	2.889136	-6.163130	-3.302427
H	1.990804	-5.594222	-3.555530
H	2.641927	-7.221078	-3.400095
H	3.644887	-5.927438	-4.049708
C	-6.222851	-2.940611	-3.291935
H	-5.661066	-2.046374	-3.573386
H	-7.282931	-2.700293	-3.383648
H	-5.992161	-3.713361	-4.023229
C	1.236822	2.060666	1.912077
C	-0.199260	2.395215	1.912860
C	-1.119319	1.504531	2.348094
C	1.669715	0.855347	2.347837
C	1.815388	2.652846	0.743464
C	0.778543	3.345566	0.023516
C	-0.457455	3.183000	0.744041

C	-1.635412	3.032787	0.056549
C	-2.328038	1.317175	1.615527
C	-1.641600	-0.776030	2.357219
C	-1.220468	-1.990945	1.940490
C	0.216143	-2.325669	1.940617
C	1.130282	-1.421197	2.356000
C	2.341916	-1.248811	1.623562
C	2.670946	0.154139	1.614385
C	3.244288	0.714900	0.501681
C	2.807071	1.999602	0.055930
C	0.778881	3.348461	-1.342533
C	1.813476	2.650491	-2.064828
C	2.802981	1.995592	-1.384462
C	3.242222	0.697758	-1.827245
C	3.513953	-0.099150	-0.658505
C	3.203912	-1.427957	-0.649083
C	2.603145	-2.020406	0.520658
C	1.644696	-2.989092	0.090887
C	0.469619	-3.132717	0.784130
C	-2.652752	-0.086772	1.624953
C	-1.811790	-2.636454	-2.022472
C	-2.798732	-1.971822	-1.347434
C	-3.239706	-0.679907	-1.805883
C	-2.671587	-0.117815	-2.918067
C	-1.636017	-0.820010	-3.630332
C	0.186068	-2.376521	-3.194663
C	0.460163	-3.166297	-2.023696
C	-0.774650	-3.325103	-1.294909
C	-0.769647	-3.305086	0.071304
C	-1.804409	-2.602243	0.784636
C	-2.797100	-1.956045	0.092485
C	-3.507333	0.133058	-0.647164
C	-3.196639	1.461709	-0.657048

C	-2.601186	2.055993	-1.825626
C	-2.344604	1.286853	-2.928279
C	-1.107461	1.449984	-3.646857
C	-0.669680	0.148236	-4.083034
C	0.663859	-0.162032	-4.083371
C	1.103176	-1.457480	-3.630975
C	1.638863	-3.003227	-1.348786
C	2.603994	-2.038209	-1.807213
C	2.343196	-1.284420	-2.919291
C	2.670058	0.120270	-2.929570
C	1.632026	0.812449	-3.647599
C	1.215927	2.047472	-3.225300
C	-0.188750	2.374501	-3.225894
C	-0.458459	3.180268	-2.064916
C	-1.634531	3.026927	-1.383584
C	-3.230693	-0.664216	0.522957
C	-2.593581	2.071998	0.502328
C	-1.218491	-2.049488	-3.193356
C	0.785805	-0.131089	3.085993
C	1.135661	-0.224540	4.571160
H	1.914066	-0.950705	4.795511
C	-0.761914	0.229373	3.086385
C	-1.115866	0.301251	4.571737
H	-0.932363	1.292017	4.987807
H	-2.135237	-0.004733	4.796977
N	-0.143537	-0.619281	5.214797
H	-0.365810	-1.570113	4.903223
C	-0.135720	-0.587594	6.686598
H	-1.116259	-0.874002	7.059731
H	0.616956	-1.278489	7.059237
H	0.100059	0.422254	7.014574
H	1.410385	0.744714	4.987660

Starting geometry of (*P*)-(12,8)-[4]CC⊃**1**$^{+}$ for MD calculations with SCC-DFTB (Fig. 4a)

C	-5.028665613233	-4.788996924189	0.434077795537
C	-4.448597334904	-5.344622597931	-0.714963738498
C	-3.237031965874	-6.083587623299	-0.661459561119
C	-2.585144047915	-6.252170625675	0.600204990578
C	-3.326854250983	-5.920598747845	1.769877958212
C	-4.511393690053	-5.216482939246	1.693053476802
C	-2.571647567917	-6.561017624537	-1.856836049304
C	-1.181254137636	-6.598234132373	0.642148208290
C	-0.471412835450	-6.751483371548	-0.578414583868
C	-1.224549701690	-6.856467419629	-1.795172653840
C	0.975169824084	-6.686044746539	-0.564463618005
C	1.658100319476	-6.482268230729	0.675957109498
C	0.922617314220	-6.579716381418	1.918586254142
C	-0.455236220002	-6.632757351720	1.877031078782
H	-4.877548619629	-5.111511804357	-1.704576332687
H	-2.936746175797	-6.167518084084	2.767823036513
H	-5.023379982415	-4.949671803705	2.629185627592
H	-0.714959612146	-7.168250116020	-2.720115204554
H	-1.007271827154	-6.646764706064	2.828817745620
C	3.009803154683	-6.054163425208	0.657935594999
H	3.481070238651	-5.776733174919	1.612003295799
C	1.756630528421	-6.655660631063	-1.755988930489
H	1.303156383428	-6.914443817793	-2.724862218748
C	3.699991009852	-5.816929114880	-0.535910722012
C	3.073550427512	-6.234388615284	-1.746455310392
H	3.618710840177	-6.190693807678	-2.701643440873
C	4.886817325756	-4.930328436849	-0.524552538626
C	5.171570040062	-4.128722714255	-1.635430658833
C	5.606151131474	-4.663486867654	0.677992268925
C	5.965111991804	-2.956183553655	-1.532287745092
H	4.670629488246	-4.339678623813	-2.592119966847

C	6.357249200287	-3.511576579966	0.810936485916
H	5.539148214593	-5.351540878083	1.534525701532
C	6.453155984003	-2.561067162083	-0.246814116680
C	6.177510645281	-2.083631290464	-2.666601084390
H	6.847296412223	-3.321039770469	1.777318282727
C	6.861075414564	-1.187729631189	-0.032596477469
C	6.653016787210	-0.806516901891	-2.450705711856
C	6.883329455064	-0.291072617245	-1.132495146379
C	7.060906915958	-0.664727484419	1.287780991557
H	6.774137308268	-0.141212544608	-3.319204278502
C	6.940229673752	1.134224724109	-0.884561030518
C	7.030051926996	0.689487725325	1.553425225803
H	7.154029130964	-1.360470752452	2.135705998778
C	6.849641052117	1.618019229110	0.458120834172
C	6.910985262976	2.100472633777	-1.931973402837
C	6.439877513879	2.960172973433	0.677399434839
H	7.139471096073	1.808002460355	-2.967769977520
C	6.538280682935	3.408071472337	-1.690932731004
H	6.216838414546	3.276548127898	1.707273467577
C	6.153729777600	3.828570731168	-0.382584415707
H	6.497991129814	4.108211089689	-2.539208365261
C	-5.921117287457	-3.611144440104	0.344417574729
C	-6.031272803421	-2.739454140471	1.434181512565
C	-6.481885430717	-3.168231101326	-0.893146479858
C	-6.451132852794	-1.393212947247	1.292820470987
H	-5.675042628293	-3.067356853012	2.420686086064
C	-6.871302213127	-1.849255019959	-1.062491331477
H	-6.623209157319	-3.875097577571	-1.727750357949
C	-6.731644852512	-0.889650352272	-0.016442689649
C	-6.467850453548	-0.486647081425	2.419885181227
H	-7.279005006554	-1.547103574864	-2.040755407745
C	-6.707540895201	0.539025273133	-0.246936248830
C	-6.536809885044	0.870353442430	2.181829118513

C	-6.527026996948	1.414293185769	0.855810955561
C	-6.665665612220	1.086148148291	-1.573177604422
H	-6.504695635284	1.552509539834	3.044472678102
C	-6.158901715807	2.794019701173	0.617541108940
C	-6.203237060640	2.363211580822	-1.823554826803
H	-6.949546047275	0.451480123324	-2.429729778651
C	-5.836270772262	3.213884261482	-0.711019623880
C	-5.940413056296	3.725423204082	1.673677844379
C	-5.071149024282	4.396175447682	-0.890004553440
H	-6.305459459955	3.512307658265	2.689225160368
C	-5.225337821772	4.889189623657	1.468453837346
H	-4.698395328652	4.632927669438	-1.897629433367
C	-4.662696524535	5.185186663600	0.192242910287
H	-5.059618597649	5.563748177294	2.321911282561
C	5.249287952315	4.984713082081	-0.181680394700
C	4.468652330256	5.441930303393	-1.249908653223
C	4.938192796425	5.489687842900	1.115022644890
C	3.284521089918	6.196670855187	-1.051926567986
H	4.707590850559	5.108853163508	-2.270388695801
C	3.780078349499	6.211887483401	1.335624205984
H	5.594429154526	5.273914337839	1.971914207838
C	2.859097355352	6.484925377445	0.282481569945
C	2.434957728381	6.568757407210	-2.162876944841
H	3.558167924322	6.529537040771	2.365393074114
C	1.483134803694	6.871273507745	0.521455153398
C	1.141156174719	6.973645159529	-1.909570034172
C	0.599876830800	7.008475300507	-0.582109479334
C	0.941869874264	6.936308738552	1.848091006074
H	0.490601726298	7.210162899135	-2.765382313611
C	-0.829767905023	6.991661122260	-0.352041555619
C	-0.414904786244	6.870551526184	2.091972855256
H	1.626158883991	6.958890238040	2.709962767897
C	-1.325893201011	6.773429448529	0.971609480709

C	-1.778532490645	7.002334734299	-1.416202429941
C	-2.662622772513	6.326804638349	1.138374199088
H	-1.475921819296	7.303363600337	-2.430128015356
C	-3.077782232374	6.571527441751	-1.228034709692
H	-2.988611389657	6.016854463617	2.142523592062
C	-3.511383660255	6.105208630987	0.047337848804
H	-3.761801525567	6.557335873964	-2.090538901956
C	-6.051921611216	2.830723379130	-3.241994360232
H	-4.988898844361	2.938027151138	-3.520442831526
H	-6.534905745973	3.805556324170	-3.407176665746
H	-6.499915029375	2.117058104786	-3.948072586907
C	-3.317862627726	-6.727064554029	-3.151631043929
H	-2.717505478536	-7.275787805059	-3.889010729892
H	-3.585055360453	-5.758347868266	-3.616436240950
H	-4.256940578256	-7.282390344612	-3.007799290717
C	1.621744621067	-6.536621244815	3.245590102700
H	2.041041548112	-5.535728527670	3.447679023493
H	2.450417107478	-7.259158962347	3.297989522821
H	0.929601717703	-6.767466814353	4.066549312229
C	5.838025434630	-2.524231409502	-4.061239981556
H	4.746990640882	-2.620150488383	-4.201639701496
H	6.288388128982	-3.498651759307	-4.306510715218
H	6.195543132565	-1.799427428333	-4.805195411611
C	7.113065663570	1.169572672499	2.973373190590
H	6.140902339542	1.556564480982	3.325943526099
H	7.851787856613	1.977030624136	3.092713487971
H	7.400584117801	0.355498837976	3.652476698108
C	2.916932323865	6.464836516819	-3.580850307948
H	3.043083247899	5.412990511487	-3.891033287965
H	3.885605436110	6.968455298343	-3.723159000972
H	2.201993017093	6.922582720728	-4.278102728831
C	-0.914103310876	6.824093729361	3.507048634727
H	-1.292097397277	5.820299510313	3.769459050353

H	-1.732695016673	7.539881240209	3.679294846338
H	-0.112355548275	7.061782405181	4.219113074920
C	-6.342192974606	-0.990499138174	3.827866819961
H	-5.330546483940	-1.385359269823	4.025709362802
H	-7.060296070785	-1.796639514915	4.042931230106
H	-6.521316737681	-0.186041216640	4.553376846554
C	-0.541053205721	0.538289031738	-2.914848921450
C	0.170935049869	-0.753109648933	-2.886962886262
C	-0.421419872030	-1.880247022300	-2.315652091613
C	-1.821213170907	0.657725999189	-2.372044837217
C	0.440626526536	1.585876012462	-2.702573748881
C	1.746554113701	0.964984151931	-2.547257160931
C	1.576706097322	-0.475178432399	-2.658336632606
C	2.354076261756	-1.340421280653	-1.854375393946
C	0.356645532137	-2.742703935382	-1.461783985324
C	-1.794278952088	-2.595911385014	-0.524914293623
C	-2.497558960684	-2.152171580107	0.595091934407
C	-3.204314218443	-0.858929621079	0.566781574590
C	-3.186164750991	-0.063825864459	-0.578719578848
C	-2.984946343493	1.357835772840	-0.457744461461
C	-2.148567813779	1.802740256697	-1.559304474545
C	-1.209811553624	2.840051279279	-1.357907349547
C	0.110628960170	2.731111902959	-1.941802480288
C	2.680009348879	1.499511049776	-1.634822831776
C	2.333454031524	2.670713489176	-0.841834883229
C	1.069241831600	3.278746385016	-0.994721168504
C	0.332957372956	3.722487486387	0.178652869141
C	-1.077035391894	3.454485248120	-0.045970772074
C	-1.894461879598	3.029057180636	1.020770129662
C	-2.865001236555	1.966477370550	0.811202928480
C	-2.907934002147	1.147524124059	2.002248636951
C	-3.064570555914	-0.251683181319	1.876227950057
C	-0.486840749044	-3.180729446170	-0.362297148067

C	-0.056718177100	-1.240169459561	3.807453842717
C	0.286058446123	-2.377183110281	3.044251845696
C	1.617327993396	-2.487429280619	2.463962214725
C	2.564071076964	-1.459059698539	2.666025102903
C	2.209577341168	-0.290294485151	3.456571337332
C	0.215881250478	1.091368988292	3.991986436539
C	-1.193913474244	0.822898202951	3.763234133152
C	-1.363546338781	-0.618724194279	3.642745596605
C	-2.285333373949	-1.147463415394	2.714804571596
C	-1.933652689526	-2.315061941871	1.921936250542
C	-0.667142164916	-2.921139886803	2.089045080209
C	1.482614228639	-3.096085119834	1.150724395943
C	2.299675646335	-2.669012342147	0.084666388032
C	3.276065453442	-1.613482099798	0.292871847829
C	3.407090324552	-1.016947037847	1.564764530639
C	3.571891384882	0.423698177165	1.675497028879
C	2.835079626437	0.873483424814	2.846171953792
C	2.153978513178	2.109859169392	2.819832952591
C	0.825130246089	2.221124841620	3.403150641400
C	-1.958072471468	1.695081727217	2.958044786373
C	-1.330789951483	2.860730664437	2.350540570332
C	0.040509954362	3.117754379540	2.568414801338
C	0.883914867083	3.556125083915	1.466625251511
C	2.189475512965	2.935884376270	1.622534392156
C	2.899812505391	2.497066608509	0.484602178007
C	3.599404785807	1.221680301568	0.511916593272
C	3.468101018090	0.607052519434	-0.797211900147
C	3.309485116285	-0.790301747401	-0.906399950282
C	0.069604851191	-3.357747314632	0.923830416789
C	1.731156907982	-2.495721692971	-1.243732283822
C	0.918856766765	-0.183956097240	4.019210634069
C	-2.677260740285	-0.540235133599	-1.945570284160
C	-3.853459692127	-0.776810632831	-2.934323005558

H	-4.783266653153	-0.253793306243	-2.638489016984
C	-1.899227324623	-1.950387632746	-1.914555977372
C	-2.706804835142	-2.846940536481	-2.891384575244
H	-2.281804879619	-2.827780647743	-3.915435973660
H	-2.756322006589	-3.900828690205	-2.566783720608
N	-4.076132685727	-2.253228367173	-2.928961749721
H	-4.568818803828	-2.497642539818	-2.023652919891
C	-4.915777162282	-2.742394903863	-4.044117993655
H	-5.066425733355	-3.827374915010	-3.944513353868
H	-5.896730654664	-2.246048201987	-4.014414020282
H	-4.439497814444	-2.534230096491	-5.013525170453
H	-3.597187635029	-0.456580210340	-3.964591765480

Global minimum of of (*P*)-(12,8)-[4]CC⊃**1**$^{+}$ for realistic rolling motions with SCC-DFTB (Fig. S5)

C	-4.716366203387	-5.069298989634	0.063174936745
C	-3.998469085266	-5.234538437781	-1.125487661827
C	-2.751178434523	-5.913430891342	-1.159592393339
C	-2.214858783327	-6.439199352935	0.058585624108
C	-3.068921330857	-6.461082675208	1.199385709400
C	-4.278520053032	-5.793115595088	1.209036944687
C	-1.951182200759	-5.965150743416	-2.363270990496
C	-0.806364642463	-6.768806031037	0.136724717033
C	0.006602313037	-6.621301452398	-1.017667503091
C	-0.623154787673	-6.329157795346	-2.272109682656
C	1.447037078856	-6.578380086819	-0.867842242956
C	2.024092480134	-6.620574396938	0.440171061456
C	1.190937876773	-6.995336028384	1.563038974102
C	-0.175838402182	-7.074237176834	1.388216098327
H	-4.345867371808	-4.717396682730	-2.034722374825
H	-2.753177851429	-6.969261105009	2.122191290495
H	-4.886419297993	-5.801342481418	2.126545076175
H	-0.017281492331	-6.319419110117	-3.190967705042

H	-0.799310409631	-7.312745981949	2.263245414414
C	3.354876108516	-6.162001175771	0.625042043838
H	3.740732943497	-6.097416902071	1.652525350701
C	2.326263311235	-6.318117825911	-1.958181111138
H	1.971661767114	-6.407600499131	-2.995880772249
C	4.125295608762	-5.661977914077	-0.433278652340
C	3.617675152550	-5.874894451878	-1.750708317052
H	4.227836545274	-5.637276832650	-2.634593063407
C	5.255367545608	-4.731987050662	-0.191673520099
C	5.839954362558	-4.020638267751	-1.247788739922
C	5.612826766906	-4.326872366848	1.129539280370
C	6.545216823211	-2.807085987089	-1.043527201222
H	5.661153361330	-4.343818052041	-2.283350319798
C	6.299920287775	-3.149192176660	1.355401616041
H	5.297667734699	-4.916211295806	2.003580604075
C	6.672059115285	-2.288055441845	0.283028831146
C	7.020673990909	-2.014824336039	-2.158175352754
H	6.492978179378	-2.856649051093	2.398325362457
C	6.984704589220	-0.886255541358	0.474610461147
C	7.333539652098	-0.687971455419	-1.948073108670
C	7.193699589422	-0.064185282202	-0.664099337934
C	6.911959155859	-0.265503939452	1.765930449306
H	7.642601500481	-0.081004266212	-2.812801067558
C	7.085283287368	1.373498822024	-0.528364899077
C	6.779977631250	1.099932683346	1.917961852354
H	6.890672785610	-0.896245414558	2.667966089480
C	6.730018961562	1.936870010596	0.737511143432
C	7.138655084022	2.254127632923	-1.648320072729
C	6.193531214396	3.251855342034	0.779295311772
H	7.542912959269	1.908626758538	-2.611413555766
C	6.617420670845	3.531715601625	-1.582262068235
H	5.777878147253	3.621938225830	1.729058826657
C	6.013467589550	4.009564441810	-0.382705511189

H	6.637930822559	4.161774716812	-2.484825246694
C	-5.704021336337	-3.970456824980	0.176092978116
C	-5.730501531664	-3.215137535104	1.353025175720
C	-6.461458777827	-3.491571039862	-0.931254279041
C	-6.285429268867	-1.912144408510	1.398399529389
H	-5.184896932178	-3.584687347930	2.233743488872
C	-7.024533832730	-2.226361207033	-0.906199162018
H	-6.592372987376	-4.116162998633	-1.828757529399
C	-6.841816620726	-1.351038420918	0.205759785416
C	-6.169778692128	-1.088437168923	2.583823805675
H	-7.584978288757	-1.887321589335	-1.792847127598
C	-7.005849407197	0.085563363222	0.109340724784
C	-6.305989126977	0.277348621085	2.455591453664
C	-6.578459992621	0.898105410957	1.192101349039
C	-7.440611584946	0.736946076704	-1.096599678291
H	-6.148337161179	0.907054616699	3.343875843371
C	-6.271954429643	2.290651955019	0.947022919277
C	-7.196641648506	2.076047632995	-1.337559396685
H	-7.997344492106	0.156431772032	-1.851257408685
C	-6.435453165585	2.835377736020	-0.364748745336
C	-5.620564010810	3.103014715076	1.917522633326
C	-5.757420476504	4.033924244184	-0.710547492551
H	-5.561485428095	2.781447181328	2.967385951598
C	-4.947585393161	4.250846318764	1.550577665778
H	-5.834421687084	4.401432068929	-1.745116401509
C	-4.903287697988	4.683293216354	0.192232332181
H	-4.377245774543	4.783338662243	2.325575044894
C	5.006591694734	5.097129687050	-0.408605984082
C	4.224162724879	5.258337062864	-1.557210534984
C	4.621044477281	5.817444429824	0.757621971207
C	2.977821131135	5.934772661104	-1.530572758128
H	4.514753907181	4.729925504502	-2.477397748704
C	3.415556968955	6.494818350563	0.804677221946

H	5.263388836370	5.813897572516	1.651562214715
C	2.508786504545	6.483089996177	-0.295269169101
C	2.113123465225	5.954993919999	-2.691214547918
H	3.140723824156	6.993646861381	1.746041559100
C	1.106738445424	6.824589413291	-0.154813750069
C	0.779999516419	6.266629306569	-2.525362189591
C	0.224712077494	6.580145347190	-1.241012266023
C	0.550525392708	7.259492888637	1.093022769400
H	0.119495869167	6.224966322366	-3.405064950469
C	-1.197861172157	6.489632540064	-0.985522592656
C	-0.805650394103	7.233066251829	1.348635131686
H	1.225431081047	7.595014335505	1.895262620897
C	-1.698756293217	6.707814558426	0.336613391726
C	-2.112879752624	6.003405097577	-1.962608159427
C	-3.009182236443	6.271817660120	0.662287152944
H	-1.805573759073	5.900290310698	-3.013850659113
C	-3.367979089531	5.545357600359	-1.609858033839
H	-3.358511961722	6.395232078658	1.697909159090
C	-3.812071795284	5.581171935339	-0.255326454795
H	-3.993250678372	5.086842806023	-2.392026051198
C	-7.680219788242	2.713034721793	-2.609172108347
H	-6.848110802542	2.953899033260	-3.296197222317
H	-8.214942584212	3.652825989358	-2.408568998957
H	-8.369008367518	2.051603592678	-3.153031199234
C	-2.518527431844	-5.558158561532	-3.693636079925
H	-1.819667368971	-5.784251034882	-4.510055487348
H	-2.719279693809	-4.470912318327	-3.734496084245
H	-3.464902106673	-6.075236160893	-3.916733143580
C	1.778090924448	-7.230848674529	2.924035687017
H	2.146614936425	-6.292388955828	3.373098149759
H	2.623781640722	-7.934789246433	2.890236004158
H	1.030347915608	-7.646019776722	3.613232276035
C	7.114876995807	-2.591996973562	-3.540932930107

H	6.116616201992	-2.781211864862	-3.972490326263
H	7.663482212217	-3.546566398566	-3.550049817661
H	7.635499388951	-1.906096864165	-4.222937172597
C	6.615407039313	1.683299882638	3.291445771257
H	5.583342059935	2.036467313437	3.462356981825
H	7.286567094527	2.540246322452	3.456037454034
H	6.832796014898	0.938312295623	4.068788784708
C	2.620397833289	5.563133745077	-4.048553242190
H	2.838077790617	4.482072033701	-4.102358567903
H	3.544594183532	6.099302140276	-4.313307691928
H	1.877816485544	5.780912233278	-4.828425942642
C	-1.316610059946	7.661718921728	2.693576901322
H	-1.661136977746	6.800285400895	3.291699886607
H	-2.161640233611	8.362186102269	2.607103222956
H	-0.531241767132	8.163373026300	3.274651949982
C	-5.821401476140	-1.684126686223	3.915810598050
H	-4.774643000401	-2.032591869663	3.943331211214
H	-6.461846548047	-2.545783080599	4.157559447663
H	-5.936841936968	-0.947267860083	4.721625903914
C	-0.438580176978	0.612208805082	-3.018450753139
C	-0.376677005032	-0.860433526812	-2.975281164384
C	-1.381280474617	-1.596003599640	-2.344405525901
C	-1.502309588730	1.296071068391	-2.428178982299
C	0.916346508073	1.113476997522	-2.879729399155
C	1.815065036174	-0.023144190399	-2.755379703640
C	1.015430932475	-1.236663549405	-2.810916556790
C	1.366071849664	-2.346892196199	-2.008768177513
C	-1.024786131152	-2.700490524352	-1.490197009477
C	-2.834849477012	-1.599805073361	-0.477590412594
C	-3.204972848221	-0.872434361209	0.652427975879
C	-3.267031757075	0.598373319027	0.608467748642
C	-2.961365257098	1.288361227971	-0.564549633250
C	-2.137993817605	2.469966154816	-0.497000740610

C	-1.244663138360	2.476664886989	-1.642710831595
C	0.066856812763	2.985298748307	-1.511421688657
C	1.169276034397	2.293994362346	-2.144123619307
C	2.933426376098	0.049050347642	-1.898650218381
C	3.185022097901	1.262125921426	-1.132458078678
C	2.317456173758	2.368162815072	-1.254264504471
C	1.916767902369	3.110587506221	-0.068575557920
C	0.524938852471	3.494083353647	-0.228081223133
C	-0.342604513456	3.496940117301	0.882281082012
C	-1.694584702208	2.977046534444	0.745072847829
C	-2.036821288779	2.278223548609	1.964106887734
C	-2.806535192044	1.095085672625	1.890824366704
C	-1.917386735964	-2.702995359874	-0.344241019009
C	-0.462275557885	-1.109374387918	3.736400591796
C	-0.700362336734	-2.290068665651	2.999707760205
C	0.410753927640	-2.991654675924	2.372114484095
C	1.725039771762	-2.491259539636	2.502209676665
C	1.968482498324	-1.277024208430	3.266098236964
C	0.829194060626	0.857331971556	3.832599602171
C	-0.561643786076	1.244264478336	3.667838729682
C	-1.361157684349	0.028663096926	3.602193976851
C	-2.464738654387	-0.043571601845	2.727119922300
C	-2.706873595105	-1.254151348291	1.959880153928
C	-1.842285721258	-2.363501859212	2.100923533127
C	-0.047204719158	-3.494377433628	1.086929076098
C	0.819965300695	-3.482307541892	-0.024026557611
C	2.174496319170	-2.975079751872	0.108963567515
C	2.620228335458	-2.484825353190	1.354366452713
C	3.414190108524	-1.268293995554	1.409827653529
C	3.015090638563	-0.522693861369	2.592589706972
C	2.954452059699	0.887011989930	2.550974460469
C	1.847154251965	1.588885604955	3.182490279873
C	-0.896245018803	2.355465504877	2.863691947772

C	0.152991762562	3.110914177537	2.193720984597
C	1.504411797653	2.731889124676	2.349850125091
C	2.400219491417	2.734959927217	1.202193652690
C	3.291422280666	1.593343505621	1.325563803986
C	3.675043012890	0.869357186902	0.176666658699
C	3.737015656687	-0.582822728025	0.219302745819
C	3.284345294697	-1.091410618132	-1.063382169081
C	2.514862058690	-2.272868419273	-1.119357545505
C	-1.438892574336	-3.101415844710	0.923953682405
C	0.324085615293	-3.089513314277	-1.333696825688
C	0.890694093163	-0.597522672256	3.874854922575
C	-2.783585919273	0.613704463667	-1.933342841037
C	-3.976308191845	0.917908041624	-2.884866243917
H	-4.572383966519	1.795977346259	-2.572339866529
C	-2.715439928330	-0.995369887265	-1.883279609244
C	-3.885588614504	-1.458838974699	-2.795551213641
H	-3.535849536675	-1.693104449946	-3.821403575650
H	-4.414440996512	-2.350809320420	-2.409066463554
N	-4.832419358231	-0.305682397642	-2.861867036705
H	-5.387772779941	-0.284352823787	-1.965065960703
C	-5.786773669050	-0.395354106157	-3.989236287474
H	-6.394606030891	-1.306031761532	-3.886278018158
H	-6.453824059343	0.477722106434	-3.984813519040
H	-5.252480277471	-0.429596725583	-4.950171838277
H	-3.633816721509	1.095037633883	-3.924434131739

TS for precession of realistic rolling motion with SCC-DFTB (Fig. S5)

C	-5.205483353895	-4.397629930729	0.534789956322
C	-4.826688840080	-5.282990816462	-0.486097514724
C	-3.672808551681	-6.102554568362	-0.368855779163
C	-2.895550875346	-6.044355572432	0.829435199065
C	-3.455554897298	-5.360847723146	1.944729817116
C	-4.563709618987	-4.551039231849	1.798762293937

C	-3.164939753378	-6.894508410218	-1.476383040410
C	-1.518790355572	-6.487357260654	0.816901257619
C	-0.933797277930	-6.856694509077	-0.423033416091
C	-1.814952589052	-7.188365250403	-1.509473256202
C	0.507997240573	-6.800397791961	-0.553827621683
C	1.304049395316	-6.502347881963	0.597118663000
C	0.684655936315	-6.459458345505	1.905192269955
C	-0.691320009757	-6.417367872391	1.983648039951
H	-5.376045214061	-5.276934453663	-1.441632969606
H	-2.951328202365	-5.378188395475	2.921687929008
H	-4.886718344075	-3.955814343239	2.665055131314
H	-1.412680557097	-7.729743890141	-2.380957227806
H	-1.160759597179	-6.302866994173	2.972251696659
C	2.654494786909	-6.112242730394	0.421446313402
H	3.220200440933	-5.777887144946	1.303280792244
C	1.168256983086	-6.846493957903	-1.816402230711
H	0.614142334804	-7.152645563619	-2.718386339249
C	3.232351355073	-5.972188359365	-0.844849040479
C	2.481407724560	-6.431788161848	-1.964372376387
H	2.928862216568	-6.438470488570	-2.970210057975
C	4.456664153695	-5.146095490439	-0.969752769365
C	4.633843564353	-4.304996762781	-2.072984476080
C	5.346811214313	-4.985611719587	0.132748114031
C	5.500770344957	-3.179673817226	-2.023386863125
H	3.991508620260	-4.439400234090	-2.957225345759
C	6.177237044572	-3.884943151930	0.213671669630
H	5.355157919368	-5.718979254980	0.953619908160
C	6.179868141707	-2.882482801782	-0.799427022199
C	5.605843057125	-2.250966318248	-3.127816104778
H	6.807662271116	-3.775282667017	1.108431179948
C	6.684070368347	-1.543860638197	-0.570759389925
C	6.174358067079	-1.011636416959	-2.912796909451
C	6.604831689474	-0.584221012452	-1.613163058624

C	7.073562379978	-1.108384404427	0.739593373514
H	6.209606859084	-0.301509484791	-3.753198473781
C	6.757298701071	0.821140178491	-1.295790977221
C	7.126812398854	0.227501266780	1.082968796765
H	7.245424848463	-1.856603079078	1.528402440082
C	6.852060703886	1.226737120393	0.072562167657
C	6.646820460852	1.850894817561	-2.274328617929
C	6.542695134940	2.569517507189	0.415734086853
H	6.728328167563	1.613304381086	-3.345641637962
C	6.380301363829	3.157651437421	-1.915249513480
H	6.474292996838	2.830408889500	1.482029402791
C	6.183132002528	3.519697229426	-0.548283774622
H	6.274555400213	3.905322499009	-2.715606104926
C	-6.003430644189	-3.176561133174	0.274023000163
C	-6.436283751427	-2.348406647794	1.317606105581
C	-6.104388218562	-2.655621882467	-1.049593072699
C	-6.724203967619	-0.973814249633	1.118780510743
H	-6.465543176244	-2.746294692307	2.342407372571
C	-6.409136413707	-1.325841134620	-1.273736185640
H	-5.882133997802	-3.296892666340	-1.920046022858
C	-6.606863705126	-0.417440756468	-0.194267673579
C	-6.998654379324	-0.092587571317	2.234288229074
H	-6.423849267678	-0.969836746747	-2.315281027197
C	-6.518372405095	1.018277574201	-0.362012052128
C	-6.889115026444	1.270748957054	2.050204932368
C	-6.531375333266	1.850825875971	0.788976243146
C	-6.247637339978	1.609511747545	-1.639860993569
H	-7.041070535570	1.926747103428	2.920741997600
C	-6.039688419782	3.210625337167	0.684588632993
C	-5.781193336008	2.901260366932	-1.767608894091
H	-6.363374016756	1.003715195527	-2.552085045488
C	-5.558449285054	3.689579773969	-0.574473424445
C	-5.843690151992	4.045305302439	1.823832835348

C	-4.751380497705	4.855587804279	-0.606711291970
H	-6.281790726614	3.771849692384	2.795228895737
C	-5.040208661472	5.170053174117	1.769326245263
H	-4.283307354334	5.143338004657	-1.559774096086
C	-4.394192757736	5.545264634873	0.557234090446
H	-4.879404668376	5.752900948846	2.689111125824
C	5.395164672069	4.719934438072	-0.177571776369
C	4.628690022614	5.381111410803	-1.145211553776
C	5.173942725124	5.089518469381	1.182939160709
C	3.526432747835	6.205878146756	-0.805055168613
H	4.805316797505	5.170453321667	-2.209756868515
C	4.095938165025	5.878103831431	1.541038898934
H	5.830818697046	4.711158689406	1.980817874645
C	3.167603260990	6.357514151317	0.571222419427
C	2.679833299709	6.786448488138	-1.825438261963
H	3.937192820304	6.080625864587	2.610873292650
C	1.834150966994	6.812833995928	0.911977528087
C	1.428972319720	7.246916386703	-1.472218492481
C	0.930689790631	7.146737110676	-0.131138874460
C	1.337597159858	6.759355504359	2.256819338074
H	0.774358027301	7.641047672085	-2.264472920683
C	-0.488506429304	7.201060517962	0.149478433834
C	-0.013625951082	6.759327278167	2.541982618938
H	2.046927508735	6.634728416496	3.089506368242
C	-0.962813096291	6.850371103902	1.452586102030
C	-1.462105542547	7.416544184881	-0.869486482359
C	-2.320173118919	6.457564642789	1.606386326715
H	-1.168210531388	7.834551215277	-1.843717223369
C	-2.779542112599	7.041911175829	-0.692842780806
H	-2.641076383327	6.033032888533	2.570065049767
C	-3.203088379790	6.426602498979	0.521473827665
H	-3.489873250286	7.186574597477	-1.521428969878
C	-5.439181370403	3.433439904349	-3.128911639151

H	-4.347587141574	3.530688795932	-3.262597252582
H	-5.883148963366	4.424746532598	-3.307138673663
H	-5.801795877847	2.763161207609	-3.920572437503
C	-4.084100136292	-7.412373420332	-2.545809465476
H	-3.527143367052	-7.885239967316	-3.366764320418
H	-4.727677658377	-6.632115523170	-2.986596316980
H	-4.760888124712	-8.173450859887	-2.126516741364
C	1.505141653889	-6.356704890648	3.156993464597
H	1.991578370705	-5.369769970162	3.243478558939
H	2.297751828632	-7.119478535018	3.190358616180
H	0.881326130672	-6.487441442217	4.051274636482
C	5.050411233427	-2.587812488867	-4.481772377267
H	3.946027252038	-2.614560212424	-4.470617798504
H	5.399721248006	-3.569052972838	-4.839064774956
H	5.345874783880	-1.840186264155	-5.230273794256
C	7.404065367030	0.616852870748	2.505858027957
H	6.500522587403	1.018658420409	2.996848535196
H	8.187917989065	1.386554671155	2.577185248604
H	7.734817737628	-0.247347542746	3.097715872599
C	3.114201182478	6.839114134683	-3.261574004435
H	3.142281989415	5.833287901887	-3.715554212374
H	4.118278459963	7.277481614300	-3.370612576070
H	2.423044909028	7.444637748801	-3.863556001422
C	-0.474010879902	6.580632632236	3.959656094108
H	-0.902102321522	5.575573243862	4.121344896977
H	-1.245320652203	7.315102016105	4.237930914636
H	0.359673612047	6.692242310250	4.666025391964
C	-7.319232502555	-0.635238086978	3.596687235306
H	-6.442483726584	-1.122800556458	4.056945741525
H	-8.130115863762	-1.379165252369	3.561723588033
H	-7.636386616031	0.165870106543	4.277518590183
C	-0.300549615351	0.143522279748	-2.969467526763
C	0.814956386545	-0.803972667494	-2.787816156679

C	0.604735485694	-2.042257025641	-2.179049063868
C	-1.586910858219	-0.181120128677	-2.536727848730
C	0.220527133562	1.482276784502	-2.763024278965
C	1.638866713266	1.379434846888	-2.459617765696
C	2.000590650551	-0.029324697140	-2.471841899819
C	2.944342234979	-0.519685461750	-1.541421968958
C	1.546026478149	-2.527323328316	-1.201208215017
C	-0.599598570763	-3.121109827740	-0.449875319230
C	-1.521363988283	-2.904215399466	0.573959820590
C	-2.638158580674	-1.960547656287	0.392328491138
C	-2.785868763362	-1.265003638136	-0.807353024545
C	-3.110823925580	0.138769903591	-0.781095903058
C	-2.377602912602	0.804872586510	-1.843553273526
C	-1.892361477195	2.118521342554	-1.651285453641
C	-0.567459338263	2.465408819806	-2.120669910934
C	2.225657723262	2.253080953332	-1.520426639542
C	1.409854209548	3.255813903672	-0.850142916134
C	0.034588904402	3.364965859912	-1.148468941761
C	-0.926707355169	3.569645698486	-0.074959984726
C	-2.119243842702	2.800044595528	-0.385698291453
C	-2.831166477917	2.152992888957	0.644719532659
C	-3.337837801848	0.805331005027	0.442980133964
C	-3.213762103025	0.080199947240	1.687715612241
C	-2.855721444874	-1.286908193207	1.658711208876
C	0.806139730438	-3.186332641885	-0.139395265653
C	0.101603818006	-1.039962480379	3.887424630570
C	0.900051494618	-2.010243536595	3.243975285468
C	2.236097466695	-1.662980234991	2.780458646330
C	2.732138036796	-0.355040327102	2.975534588395
C	1.909518235423	0.642208412556	3.642707360378
C	-0.487920030041	1.238859557452	3.913894285982
C	-1.681849698537	0.472326640994	3.597348354770
C	-1.317211178179	-0.937598621182	3.574607971633

C	-1.894631626138	-1.801815634635	2.620782961778
C	-1.072789103727	-2.795037286857	1.948735701392
C	0.301660356520	-2.899634535368	2.261190260728
C	2.461095473497	-2.341434823982	1.513256442347
C	3.173406588658	-1.694065256947	0.483469654947
C	3.686364165950	-0.349160144126	0.684686948065
C	3.471691457495	0.311174195631	1.912932110110
C	3.106370376501	1.719423831571	1.924432003913
C	2.141999149926	1.924336618102	2.994840472544
C	1.072994669151	2.829405137041	2.819542042309
C	-0.260865416824	2.483961444038	3.288118896783
C	-2.620308901013	0.974338148416	2.669900869413
C	-2.386015258258	2.258600361547	2.023949636925
C	-1.223643613606	2.999907849036	2.326871187113
C	-0.483228267927	3.657509665650	1.261226257122
C	0.933124338914	3.552543308973	1.566231172067
C	1.864277108170	3.352729198678	0.525903381924
C	2.965828446417	2.420427222345	0.707310239585
C	3.189693916760	1.741674644902	-0.556684821824
C	3.543960284270	0.377167319204	-0.567878812355
C	1.259027648859	-3.097915470051	1.195691356100
C	2.710958807748	-1.790839936321	-0.892748485949
C	0.614413368419	0.303782007542	4.093188304167
C	-2.003367715523	-1.587348114586	-2.088158932091
C	-2.910131169562	-2.267528625406	-3.151806805250
H	-3.990434012190	-2.107557107882	-2.977952486081
C	-0.784799088784	-2.622693859650	-1.890064676194
C	-1.115487336487	-3.793048116479	-2.858313625416
H	-0.606693160583	-3.672640832008	-3.836060072031
H	-0.842844431532	-4.786551574288	-2.456372823126
N	-2.592392168015	-3.724953350303	-3.074271540908
H	-3.059461946460	-4.114017775622	-2.214603441748
C	-3.058475356744	-4.495409486981	-4.247557322737

H	-2.709345187929	-5.534918107825	-4.171720504384
H	-4.157702006688	-4.485521084985	-4.282152015824
H	-2.667167001485	-4.059654127325	-5.178736660662
H	-2.678396740072	-1.907650322200	-4.174716300959

TS for spin of realistic rolling motion with SCC-DFTB (Fig. S5)

C	-5.452030546871	-4.321871081610	0.885360430029
C	-4.726743962967	-4.814394220922	-0.204986924854
C	-3.551440589559	-5.593695486569	-0.035611033951
C	-3.090205358216	-5.869471327661	1.290339474045
C	-3.962333080325	-5.551222418303	2.371558596632
C	-5.105962429874	-4.799479860934	2.181362110909
C	-2.743971282877	-6.008332503155	-1.161463428530
C	-1.724740774458	-6.307992977760	1.495910351839
C	-0.890754772854	-6.545379478224	0.371466081845
C	-1.469016657178	-6.488431807192	-0.939023898359
C	0.542528878299	-6.647777204853	0.558889808240
C	1.100996947685	-6.400417216620	1.851950156830
C	0.224047692954	-6.348349435400	3.001609714558
C	-1.141812878745	-6.333959720492	2.805548883662
H	-5.007752013474	-4.491790114994	-1.222266037993
H	-3.713346152855	-5.860647626849	3.397059518575
H	-5.729473411510	-4.544432003014	3.051576221678
H	-0.857305277045	-6.764471125033	-1.811661911472
H	-1.793217006100	-6.255649389924	3.688930491174
C	2.479735644758	-6.080922949823	1.957814928288
H	2.863545728406	-5.756884064703	2.935958932376
C	1.454149140744	-6.824055766012	-0.522449927645
H	1.093656668626	-7.159466558410	-1.506664869670
C	3.318395934007	-6.018587446668	0.838290664447
C	2.796901037871	-6.526612300546	-0.388968443102
H	3.448441215413	-6.648559283302	-1.267436603096
C	4.565271406658	-5.218866575930	0.882892085654

C	5.098466586701	-4.682442032755	-0.295301568461
C	5.106634090130	-4.744158506221	2.114986231248
C	5.960805324226	-3.555255950377	-0.288775395170
H	4.748287482933	-5.062137710438	-1.266394838763
C	5.929460516187	-3.634532034913	2.147648227992
H	4.840344246833	-5.226578734352	3.067666637305
C	6.276256292232	-2.929672969257	0.958223152676
C	6.413005445901	-2.943880991550	-1.519820019205
H	6.271831690978	-3.273601050234	3.128934212069
C	6.766061916855	-1.566496764313	0.967255216327
C	6.936006454664	-1.667865831297	-1.481262032201
C	7.005673115258	-0.907902786701	-0.267267235585
C	6.839551734619	-0.803558157228	2.179820212579
H	7.235305536118	-1.197811615760	-2.430500479157
C	7.124271818507	0.535204237137	-0.290024373671
C	6.878191924733	0.576380158915	2.177303522506
H	6.777044664777	-1.322099524810	3.148827823960
C	6.898260283504	1.277750414354	0.911334800796
C	7.284644386518	1.275338293572	-1.497786109809
C	6.554674380252	2.652381718889	0.814144721904
H	7.615380812606	0.774205429805	-2.419770956757
C	6.969752648920	2.618493553847	-1.563444445409
H	6.223556090075	3.175549720011	1.723855078485
C	6.461576753190	3.304675490000	-0.420763637584
H	7.074554229619	3.139391175306	-2.527492518327
C	-6.323596306733	-3.138227369728	0.699910669175
C	-6.289381984589	-2.123469747222	1.661877301940
C	-6.980691183545	-2.854643195282	-0.533797494006
C	-6.638615874387	-0.784726805997	1.349708563328
H	-5.844660360211	-2.336628297224	2.645346566748
C	-7.317125533222	-1.552884669796	-0.864654625034
H	-7.197225420882	-3.664639311376	-1.248571781989
C	-7.000156901955	-0.464985812457	0.003064119591

C	-6.486670199319	0.282781195283	2.314512769981
H	-7.781956963079	-1.365242176621	-1.845675155054
C	-6.838701625781	0.897588163950	-0.461335644379
C	-6.462815748406	1.587492784579	1.866936727855
C	-6.494671519391	1.910661410328	0.470128530376
C	-6.787718889072	1.206220464579	-1.862614143060
H	-6.302377009593	2.389473870389	2.603072348948
C	-6.000786731390	3.183179788408	-0.011224395698
C	-6.182282993998	2.353279272028	-2.338267435759
H	-7.170472971651	0.472494013628	-2.592278358147
C	-5.687829467454	3.336753004368	-1.398142037042
C	-5.663639869521	4.257794520137	0.860775972413
C	-4.818774874673	4.388588130301	-1.792939381105
H	-6.017540103106	4.261735170090	1.902310722468
C	-4.855455925770	5.295772962291	0.441639109396
H	-4.467133180936	4.412009765950	-2.835004101417
C	-4.300974595783	5.309631177713	-0.873182964915
H	-4.609909987928	6.089916957963	1.162294509181
C	5.619926860065	4.516108035476	-0.560780326303
C	4.938470603970	4.738970417603	-1.762775632382
C	5.260594280948	5.326672954663	0.555015150696
C	3.790508895935	5.568979849097	-1.836553660970
H	5.218143841338	4.155256668862	-2.652178966606
C	4.141685948668	6.137582226284	0.509674396517
H	5.847113305026	5.287493443647	1.485658406750
C	3.306274659131	6.192677534804	-0.644197975636
C	3.022000497012	5.681831353647	-3.057831589740
H	3.876944331211	6.702198445019	1.416085020633
C	1.943399985428	6.684131334242	-0.601702103995
C	1.736906764965	6.179394468638	-2.997062471326
C	1.127728510462	6.569472410467	-1.758936095151
C	1.340214967276	7.117214669585	0.624969824099
H	1.145314094223	6.212638135153	-3.924773566324

C	-0.310435626026	6.672802316167	-1.624729881553
C	-0.028197051739	7.192433693632	0.785985128088
H	1.979869759653	7.333845007704	1.494060340244
C	-0.886106602905	6.846673838034	-0.327296956167
C	-1.204101231844	6.440407279075	-2.710786746473
C	-2.257697237563	6.537805702540	-0.135972269312
H	-0.832521084020	6.431811341532	-3.746301252397
C	-2.539062979345	6.152211505907	-2.499907266626
H	-2.650184905629	6.541965130305	0.891285717825
C	-3.071600611306	6.078019442405	-1.178838312010
H	-3.174367504877	5.939424002135	-3.373372979955
C	-6.017970722220	2.540920011983	-3.819429537592
H	-4.956058323657	2.485551153377	-4.119766547056
H	-6.403796057549	3.514502324951	-4.157302191403
H	-6.552164867846	1.762016577951	-4.383049765921
C	-3.248682645353	-5.879530616257	-2.571674711902
H	-2.566368405936	-6.358360138718	-3.286659714748
H	-3.338243617315	-4.816229337838	-2.882204307770
H	-4.241128111305	-6.337947522189	-2.703369427821
C	0.772291352584	-6.249206478810	4.395018138808
H	1.247078081000	-5.268705354736	4.572028946252
H	1.528599783033	-7.023530912859	4.595754412670
H	-0.022971506238	-6.362213935169	5.144100185757
C	6.267205197918	-3.647599510839	-2.838118976599
H	5.208557577513	-3.724981002860	-3.142125707643
H	6.676145421313	-4.669436547301	-2.806504066402
H	6.792542298471	-3.107122398915	-3.637231111913
C	6.825730511008	1.323529327595	3.478266663612
H	5.847559802793	1.815269453967	3.621985116891
H	7.598632866713	2.105323727124	3.535636771821
H	6.974569005524	0.647978474890	4.331511015984
C	3.570683244224	5.201901685555	-4.370229937830
H	3.649974371021	4.101044455063	-4.397936523749

H	4.573449047231	5.609624752992	-4.570818870649
H	2.921151677514	5.498802344351	-5.205057930727
C	-0.599241670232	7.556106037444	2.125927024625
H	-1.061308882601	6.683146066841	2.619354242385
H	-1.371205190264	8.337115565551	2.046660958132
H	0.181264664702	7.931389162853	2.801421046945
C	-6.282798685897	-0.010026959994	3.772093034291
H	-5.286167162790	-0.446899078024	3.958270476511
H	-7.031459221942	-0.718027236821	4.159060473134
H	-6.350247456128	0.905969678961	4.373931073213
C	-2.778992194639	1.608001021482	-0.883946033873
C	-1.825426773630	1.824102750369	-1.988028071908
C	-1.357160368101	0.749766142054	-2.746948930173
C	-3.229690314351	0.325738624051	-0.574378653148
C	-2.436645605880	2.530863616285	0.180881178219
C	-1.289650004275	3.312595995792	-0.245095120570
C	-0.913916279514	2.876341367437	-1.579187223319
C	0.451987645395	2.820423840456	-1.939321614337
C	0.044543627721	0.666592285416	-3.077406660389
C	-0.682097481683	-1.516606816483	-2.598371544414
C	-0.513494273374	-2.580478394962	-1.710943722416
C	-1.468953717100	-2.793033833107	-0.607696321999
C	-2.555818738801	-1.936845221531	-0.434888483113
C	-2.903686079962	-1.481895685443	0.888252417979
C	-3.315090365149	-0.091570149854	0.801741223539
C	-3.008475338785	0.803834904187	1.850584788024
C	-2.561180122534	2.143254307187	1.534286859003
C	-0.297719965914	3.677792504907	0.687097803100
C	-0.419224424069	3.270742535838	2.078816895562
C	-1.535734274378	2.514237733710	2.497074236134
C	-1.353474599249	1.395679279639	3.411407094638
C	-2.267941101415	0.336251493132	3.013463183235
C	-1.867274790070	-1.014034641153	3.098230961070

C	-2.195064543911	-1.939415169937	2.022449419906
C	-1.077722189073	-2.841469693612	1.846207861649
C	-0.714967309754	-3.248578541062	0.543079546319
C	0.458342865916	-0.724037911749	-2.988031148333
C	2.836240115446	-2.203825769492	0.681232950730
C	2.964900429239	-1.802911665472	-0.665487919421
C	3.423662839885	-0.458577052909	-0.981958314889
C	3.735492619291	0.439982783793	0.060259230941
C	3.610489364049	0.021006140552	1.446537685885
C	2.229246809218	-1.498518161519	2.842837764250
C	1.312027434207	-2.552769917649	2.443490456761
C	1.683903584063	-2.983656050664	1.103712984727
C	0.686136808088	-3.327572001380	0.170296673561
C	0.809604432009	-2.913443066969	-1.216622809562
C	1.936357878456	-2.164331930326	-1.627645789781
C	2.677717520231	0.009849192847	-2.139420362180
C	2.275391152792	1.359392749612	-2.223505322747
C	2.605033741767	2.285941310375	-1.152448891926
C	3.324004006323	1.831977704703	-0.026554020412
C	2.947253483148	2.274220359468	1.306897693488
C	3.126293792580	1.154304833903	2.218790563036
C	2.211216914301	0.947473576292	3.273523491666
C	1.756563879371	-0.398285139649	3.591066268356
C	-0.049610324249	-2.483899817982	2.810541012262
C	-0.537392135593	-1.350726892059	3.583895947638
C	0.352747300810	-0.322804649004	3.965327489595
C	-0.061224727112	1.070110544066	3.878118310712
C	1.087021024496	1.854496667305	3.450395290744
C	0.910288198518	2.939943471394	2.564772659116
C	1.855083787501	3.152432630548	1.476224912856
C	1.107362821372	3.608631161411	0.318026210438
C	1.476505352121	3.186344163438	-0.975871761548
C	1.756574999086	-1.047939385319	-2.531302767932

C	0.941353020700	1.693388501603	-2.704031682588
C	3.171660003492	-1.284224082272	1.753322135835
C	-2.996206102317	-0.893090426427	-1.470257015118
C	-4.302540353417	-1.320855650070	-2.182689041881
H	-4.896053075467	-2.058833886983	-1.609585059675
C	-1.955176490653	-0.660622577183	-2.678698770727
C	-2.782094021449	-0.999670587573	-3.955868417900
H	-3.249527775708	-0.096112014925	-4.397436782039
H	-2.190369284931	-1.496380461223	-4.748303936459
N	-3.862922532918	-1.914188937341	-3.478204436194
H	-3.424176120349	-2.848099593029	-3.267764352635
C	-4.963746070792	-2.134309783069	-4.440716791237
H	-4.566624019427	-2.578186316840	-5.365402191867
H	-5.700244093364	-2.824030197153	-4.002345926974
H	-5.464478936601	-1.185071114214	-4.683100127049
H	-4.953895524560	-0.447998082754	-2.393664316338

1/2 spin of (*P*)-(12,8)-[4]CC⊃**1**$^{+}$ during realistic rolling motions with SCC-DFTB (Fig. S5)

C	-2.179779832718	3.930840192774	-3.952649888144
C	-3.094474894900	4.146621836216	-2.917009898194
C	-2.759960439847	4.919891211696	-1.772400477645
C	-1.442986039563	5.470318070177	-1.670304946715
C	-0.621077866310	5.434175659718	-2.834018105179
C	-0.973414215386	4.688408279904	-3.942207342582
C	-3.665046589327	5.051592243076	-0.651965988918
C	-0.939604047543	5.884157118295	-0.376525560542
C	-1.795228223872	5.825228097874	0.754430555280
C	-3.180854286139	5.515911203935	0.554296321822
C	-1.219413123941	5.884091369553	2.082721882613
C	0.202832907173	5.897372091168	2.233992116642
C	1.030516721280	6.161922760623	1.076655718220
C	0.450205868902	6.175870792363	-0.175472955300

H	-4.051521481234	3.599526317544	-2.928172719956
H	0.342485102516	5.964083247005	-2.852635279908
H	-0.290957369530	4.658002434247	-4.805213341459
H	-3.874563313624	5.570288694687	1.407266839766
H	1.100564926233	6.336447245716	-1.048662527316
C	0.768039086487	5.516741279149	3.479300609281
H	1.859854232331	5.400482231111	3.537918480508
C	-1.998688648292	5.759317007728	3.269169636005
H	-3.090664385314	5.891015633616	3.236067985635
C	-0.022672046148	5.146864184458	4.574738002394
C	-1.422444080941	5.409934036251	4.474916697697
H	-2.080857121763	5.290104566815	5.348251032789
C	0.525200411581	4.288252497543	5.652392634627
C	-0.334881920253	3.565934472698	6.489085936891
C	1.912201658862	3.957576829733	5.715078701798
C	0.087651594678	2.408127364374	7.191062712973
H	-1.401842650301	3.829322639801	6.524233120630
C	2.345412135406	2.823434153268	6.375917902420
H	2.660783078253	4.572971884686	5.193651309245
C	1.430628355710	1.945074015086	7.025944933030
C	-0.842596567648	1.614029057463	7.965052167327
H	3.418505062558	2.583020242929	6.340135257079
C	1.754726381577	0.570898693459	7.353294384393
C	-0.492341643808	0.326921221389	8.315622652090
C	0.748322729713	-0.264558005672	7.905470651814
C	3.000409863965	-0.021989317247	6.960176687808
H	-1.225872615523	-0.282279547185	8.865518275697
C	0.919130651957	-1.701993232255	7.866440116862
C	3.165083377696	-1.389095297371	6.862855430550
H	3.832365082855	0.627547412154	6.647294435437
C	2.058691444044	-2.257796792207	7.204429702455
C	-0.093738669062	-2.605972365935	8.302172062664
C	2.006509622327	-3.607828014415	6.763567781932

H	-0.913297333455	-2.257305772095	8.948051127361
C	-0.117542702541	-3.917819801751	7.870988867255
H	2.814719437110	-3.983216689875	6.117341716616
C	0.877551174851	-4.406588213347	6.974333816748
H	-0.942556246633	-4.569767444008	8.197059486892
C	-2.342772866350	2.762467748587	-4.849516109306
C	-1.207689451356	2.013927349274	-5.177079695176
C	-3.612534153987	2.221334380259	-5.200050029629
C	-1.294324918847	0.673985766171	-5.629743101041
H	-0.214644975737	2.427770679680	-4.947717754151
C	-3.722731753600	0.915013480588	-5.649521067790
H	-4.525597752942	2.827381574172	-5.090134410508
C	-2.582264752512	0.064587032720	-5.758945772805
C	-0.104728067803	-0.128163789433	-5.824413776712
H	-4.728012237382	0.529123588879	-5.884883624610
C	-2.679908713192	-1.380354047489	-5.795865052770
C	-0.227002659034	-1.501102310475	-5.836073063441
C	-1.494602824662	-2.151801855428	-5.674821784981
C	-3.939680124550	-2.069357121516	-5.785335869026
H	0.686614928411	-2.108732866870	-5.917444222606
C	-1.590506356892	-3.523795246862	-5.225379167416
C	-4.056009663835	-3.387450021643	-5.385343804106
H	-4.851509367395	-1.528566330573	-6.088331286176
C	-2.870560933040	-4.092494334023	-4.937504841305
C	-0.440207731918	-4.278127889656	-4.859102679525
C	-2.949199422015	-5.247343468083	-4.114719912780
H	0.565521757734	-3.941507334461	-5.149439685908
C	-0.542639075687	-5.383012717549	-4.038639650559
H	-3.944163752427	-5.629610684867	-3.840658920120
C	-1.805806179353	-5.829476108199	-3.549361974081
H	0.388239681345	-5.866514953675	-3.708410458170
C	0.608337641394	-5.562352905041	6.086282611456
C	-0.711983662366	-5.813488358181	5.697345960468

C	1.640497059029	-6.270849747965	5.407692295576
C	-1.025757166357	-6.574611619193	4.542536080187
H	-1.528811292052	-5.295058522796	6.221136236574
C	1.358534799862	-7.028947560002	4.285112847997
H	2.684570372664	-6.194440511034	5.748011280908
C	0.038320717336	-7.115911586363	3.754297132893
C	-2.389750998322	-6.691557045815	4.072312788623
H	2.198554484637	-7.515665307629	3.767408482152
C	-0.231205731848	-7.551694250927	2.398018001828
C	-2.615698905514	-7.091079436813	2.771941165303
C	-1.542917132141	-7.404010053088	1.873425619695
C	0.812462499030	-7.987350247234	1.516786101071
H	-3.653911966000	-7.123309737194	2.407244060003
C	-1.731307728620	-7.408170741927	0.437462571659
C	0.647287943273	-8.050417371302	0.147855788548
H	1.796098396624	-8.249394533611	1.935682856713
C	-0.611139440993	-7.620729154416	-0.426219097183
C	-2.960479118838	-7.016852615442	-0.166253885807
C	-0.715573075277	-7.268130701372	-1.796637674063
H	-3.875450595372	-6.925132919816	0.437748291268
C	-3.022652392610	-6.635458800878	-1.493011186781
H	0.172945386057	-7.385416558427	-2.434084213429
C	-1.863560616676	-6.660901238305	-2.323056058842
H	-3.978514522850	-6.246639144750	-1.877695397165
C	-5.409305600268	-4.039784102713	-5.355357895015
H	-5.767620300086	-4.197339020006	-4.320897743782
H	-5.397921456807	-5.022698510644	-5.848544845430
H	-6.162167399346	-3.422337476604	-5.865062015817
C	-5.103948882737	4.632886550095	-0.759888626666
H	-5.676212953887	4.942558312191	0.124876533273
H	-5.202941583676	3.533539311640	-0.836845768392
H	-5.598140878807	5.068896272789	-1.642054676011
C	2.512786504343	6.357051804221	1.208239382220

H	3.019821368027	5.417845842388	1.489539674414
H	2.762397292258	7.108601560839	1.972943599424
H	2.955692720815	6.690903785945	0.260165617358
C	-2.195986858842	2.144996767838	8.339991823377
H	-2.853031380020	2.243228280098	7.458297484789
H	-2.131046934694	3.136682066334	8.814015096841
H	-2.703894724073	1.474631121157	9.046620296230
C	4.457076486859	-1.946599066061	6.339542129123
H	4.337396970835	-2.363640235877	5.324191628422
H	4.846657025624	-2.751882974391	6.981187903118
H	5.230302159950	-1.168851143288	6.278289407161
C	-3.550566222331	-6.307015665956	4.943016460628
H	-3.591149149705	-5.215540639413	5.104631627994
H	-3.498918252830	-6.785322516283	5.933110508852
H	-4.505197302394	-6.599935172132	4.484744755383
C	1.796520903938	-8.474078675129	-0.720170696295
H	2.220193082923	-7.621848884641	-1.279360513164
H	1.495324314749	-9.234800842905	-1.456906216499
H	2.610621859214	-8.901491726773	-0.119569513274
C	1.253159022209	0.502021684266	-5.924249558513
H	1.579178620911	0.917803099090	-4.955221983250
H	1.270806602796	1.322415392781	-6.657650385931
H	2.009516114635	-0.233035532602	-6.229878971779
C	-0.959302327680	-0.050444475608	-2.400205878767
C	-0.957641659466	-1.523277735273	-2.403581579202
C	-1.989183633699	-2.238622713727	-1.796100209664
C	-1.992178895073	0.660503015128	-1.789882995491
C	0.414362740280	0.391060139103	-2.253220279845
C	1.265135831464	-0.784948636151	-2.168243879686
C	0.416940623991	-1.962201657828	-2.258600276518
C	0.723749337808	-3.110758375970	-1.493336817359
C	-1.676707013447	-3.382746541240	-0.978351908815
C	-3.437831174942	-2.239580199254	0.075584591964

C	-3.777890455810	-1.534158936276	1.231062005354
C	-3.779461665088	-0.058976554595	1.234158676760
C	-3.441364525802	0.651965435168	0.081392813469
C	-2.571804993607	1.797545639810	0.180871122049
C	-1.681004296922	1.800710513341	-0.966628246787
C	-0.350847718693	2.255144402768	-0.827054337908
C	0.719398328497	1.537893050467	-1.484751133091
C	2.385958642203	-0.785537067617	-1.312160852828
C	2.691308805407	0.391417358339	-0.510529978380
C	1.872651755992	1.538277823203	-0.597324797913
C	1.509227205827	2.264216970616	0.611685624215
C	0.131839145696	2.706574345646	0.469070495528
C	-0.731711241067	2.698946584527	1.582882798982
C	-2.106217737884	2.246245641751	1.437118913974
C	-2.474769921937	1.525461060061	2.636255893708
C	-3.293952773969	0.377908884160	2.530294257633
C	-2.567529203845	-3.385517196333	0.169412719126
C	-1.037057179296	-1.978630429868	4.297092272118
C	-1.323730017477	-3.121892162285	3.521261550010
C	-0.244069434998	-3.843047412381	2.864338142504
C	1.090392727496	-3.409269991141	3.008099267391
C	1.382869885074	-2.229595937083	3.805201044740
C	0.334154008905	-0.072237384093	4.440674318311
C	-1.039268125885	0.378199201872	4.301609112930
C	-1.889119117433	-0.800704130066	4.203338046855
C	-2.996424352680	-0.800155904558	3.329389864054
C	-3.291691722055	-1.975509572723	2.525407877687
C	-2.469741724260	-3.121384975809	2.625722694796
C	-0.724293243929	-4.287955199872	1.567781864803
C	0.139324885597	-4.291935421863	0.454212245966
C	1.515579785283	-3.845588138575	0.599143177022
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