Electronic Supplementary Material for PCCP

Supporting information

for

Weak distance dependence of through-bond interactions in tetrahydro-*4H*-thiopyran-4-ylidene end-capped oligo(cyclohexylidenes); a computational survey

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Table S1. RHF/6-31G* optimised Cartesian coordinates of **1(1)**.

Atom	X	Y	Z
C	-0.372214	-1.202923	0.000000
C	0.372214	1.202923	0.000000
C	0.835888	2.780442	2.355140
C	-0.835888	-2.780442	-2.355140
C	0.835888	2.780442	-2.355140
C	-0.835888	-2.780442	2.355140
C	-0.835888	5.154614	2.383387
C	0.835888	-5.154614	-2.383387
C	-0.835888	5.154614	-2.383387
C	0.835888	-5.154614	2.383387
C	-0.462987	6.745599	0.000000
C	0.462987	-6.745599	0.000000
H	2.809399	3.372935	2.360476
H	-2.809399	-3.372935	-2.360476
H	2.809399	3.372935	-2.360476
H	-2.809399	-3.372935	2.360476
H	0.547592	1.729294	4.079472
H	-0.547592	-1.729294	-4.079472
H	0.547592	1.729294	-4.079472
H	-0.547592	-1.729294	4.079472
H	-2.805710	4.582416	2.525849
H	2.805710	-4.582416	-2.525849
H	-2.805710	4.582416	-2.525849
H	2.805710	-4.582416	2.525849
H	-0.419281	6.274251	4.054388
H	0.419281	-6.274251	-4.054388
H	-0.419281	6.274251	-4.054388
H	0.419281	-6.274251	4.054388
H	1.440337	7.528547	0.000000
H	-1.440337	-7.528547	0.000000
H	-1.754992	8.342075	0.000000
H	1.754992	-8.342075	0.000000

Table S2. RHF/6-31G* optimised Cartesian coordinates of **1(2)**.

Atom	X	Y	Z
C	0.792019	1.222426	2.347736
C	-0.792019	-1.222426	-2.347736
C	0.792019	1.222426	-2.347736
C	-0.792019	-1.222426	2.347736
C	-0.318641	-2.797900	0.000000
C	0.318641	2.797900	0.000000
C	0.428868	-5.202684	0.000000
C	-0.428868	5.202684	0.000000
C	0.887368	-6.781308	2.354891
C	-0.887368	6.781308	-2.354891
C	0.887368	-6.781308	-2.354891
C	-0.887368	6.781308	2.354891
C	-0.792019	-9.150659	2.383229
C	0.792019	9.150659	-2.383229
C	-0.792019	-9.150659	-2.383229
C	0.792019	9.150659	2.383229
C	-0.424403	-10.743109	0.000000
C	0.424403	10.743109	0.000000
H	2.782493	0.698150	2.396397
H	-2.782493	-0.698150	-2.396397
H	2.782493	0.698150	-2.396397
H	-2.782493	-0.698150	2.396397
H	2.858879	-7.380426	2.360508
H	-2.858879	7.380426	-2.360508
H	2.858879	-7.380426	-2.360508
H	-2.858879	7.380426	2.360508
H	-2.759984	-8.572421	2.526070
H	2.759984	8.572421	-2.526070
H	-2.759984	-8.572421	-2.526070
H	2.759984	8.572421	2.526070
H	1.476372	-11.532134	0.000000
H	-1.476372	11.532134	0.000000
H	0.415974	2.245663	4.072203
H	-0.415974	-2.245663	-4.072203
H	0.415974	2.245663	-4.072203
H	-0.415974	-2.245663	4.072203
H	0.600630	-5.729711	4.079250
H	-0.600630	5.729711	-4.079250
H	0.600630	-5.729711	-4.079250
H	-0.600630	5.729711	4.079250
H	-0.377927	-10.271135	4.054233
H	0.377927	10.271135	-4.054233
H	-0.377927	-10.271135	-4.054233
H	0.377927	10.271135	4.054233
H	-1.721571	-12.335285	0.000000
H	1.721571	12.335285	0.000000

Table S3. RHF/6-31G* optimised Cartesian coordinates of **1(3)**.

Atom	X	Y	Z
C	0.013756	-1.258919	0.000000
C	-0.013756	1.258919	0.000000
C	-0.005613	2.904141	2.347694
C	0.005613	-2.904141	-2.347694
C	-0.005613	2.904141	-2.347694
C	0.005613	-2.904141	2.347694
C	2.231595	4.770343	2.347179
C	-2.231595	-4.770343	-2.347179
C	2.231595	4.770343	-2.347179
C	-2.231595	-4.770343	2.347179
C	2.238779	6.416306	0.000000
C	-2.238779	-6.416306	0.000000
C	2.215481	8.934352	0.000000
C	-2.215481	-8.934352	0.000000
C	2.231595	10.578332	2.354655
C	-2.231595	-10.578332	-2.354655
C	2.231595	10.578332	-2.354655
C	-2.231595	-10.578332	2.354655
C	4.523160	12.362119	2.383381
C	-4.523160	-12.362119	-2.383381
C	4.523160	12.362119	-2.383381
C	-4.523160	-12.362119	2.383381
C	4.631941	13.992877	0.000000
C	-4.631941	-13.992877	0.000000
H	-1.751737	3.993857	2.394114
H	1.751737	-3.993857	-2.394114
H	-1.751737	3.993857	-2.394114
H	1.751737	-3.993857	2.394114
H	3.977923	3.680919	2.391713
H	-3.977923	-3.680919	-2.391713
H	3.977923	3.680919	-2.391713
H	-3.977923	-3.680919	2.391713
H	0.516595	11.720500	2.360622
H	-0.516595	-11.720500	-2.360622
H	0.516595	11.720500	-2.360622
H	-0.516595	-11.720500	2.360622
H	6.240219	11.240128	2.526498
H	-6.240219	-11.240128	-2.526498
H	6.240219	11.240128	-2.526498
H	-6.240219	-11.240128	2.526498
H	0.050676	1.815502	4.072318
H	-0.050676	-1.815502	-4.072318
H	0.050676	1.815502	-4.072318
H	-0.050676	-1.815502	4.072318
H	2.177783	5.857948	4.072480
H	-2.177783	-5.857948	-4.072480
H	2.177783	5.857948	-4.072480
H	-2.177783	-5.857948	4.072480
H	2.202704	9.488622	4.079034
H	-2.202704	-9.488622	-4.079034
H	2.202704	9.488622	-4.079034

H	-2.202704	-9.488622	4.079034
H	4.450168	13.554255	4.054501
H	-4.450168	-13.554255	-4.054501
H	4.450168	13.554255	-4.054501
H	-4.450168	-13.554255	4.054501
H	3.041440	15.298896	0.000000
H	-3.041440	-15.298896	0.000000
H	6.334800	15.140942	0.000000
H	-6.334800	-15.140942	0.000000

Table S4. RHF/6-31G* optimised Cartesian coordinates of **1(4)**.

Atom	X	Y	Z
C	-0.799795	-1.217497	2.347345
C	0.799795	1.217497	-2.347345
C	-0.799795	-1.217497	-2.347345
C	0.799795	1.217497	2.347345
C	0.330587	2.794979	0.000000
C	-0.330587	-2.794979	0.000000
C	-0.422653	5.197776	0.000000
C	0.422653	-5.197776	0.000000
C	-0.890586	6.775062	2.347667
C	0.890586	-6.775062	-2.347667
C	-0.890586	6.775062	-2.347667
C	0.890586	-6.775062	2.347667
C	0.708147	9.210599	2.347308
C	-0.708147	-9.210599	-2.347308
C	0.708147	9.210599	-2.347308
C	-0.708147	-9.210599	2.347308
C	0.239518	10.788673	0.000000
C	-0.239518	-10.788673	0.000000
C	0.505506	-13.194144	0.000000
C	-0.505506	13.194144	0.000000
C	-0.966256	14.772106	2.355222
C	0.966256	-14.772106	-2.355222
C	-0.966256	14.772106	-2.355222
C	0.966256	-14.772106	2.355222
C	0.704284	17.147489	2.382790
C	-0.704284	-17.147489	-2.382790
C	0.704284	17.147489	-2.382790
C	-0.704284	-17.147489	2.382790
C	0.329607	18.738904	0.000000
C	-0.329607	-18.738904	0.000000
H	-2.786985	-0.681191	2.393114
H	2.786985	0.681191	-2.393114
H	-2.786985	-0.681191	-2.393114
H	2.786985	0.681191	2.393114
H	-2.877980	7.310796	2.394472
H	2.877980	-7.310796	-2.394472
H	-2.877980	7.310796	-2.394472
H	2.877980	-7.310796	2.394472
H	2.695514	8.674761	2.392855
H	-2.695514	-8.674761	-2.392855
H	2.695514	8.674761	-2.392855
H	-2.695514	-8.674761	2.392855
H	-0.430607	-2.242599	4.072332
H	0.430607	2.242599	-4.072332
H	-0.430607	-2.242599	-4.072332
H	0.430607	2.242599	4.072332
H	-0.520505	5.749847	4.072413
H	0.520505	-5.749847	-4.072413
H	-0.520505	5.749847	-4.072413
H	0.520505	-5.749847	4.072413
H	0.340278	10.235484	4.072618

H	-0.340278	-10.235484	-4.072618
H	0.340278	10.235484	-4.072618
H	-0.340278	-10.235484	4.072618
H	1.574511	-19.519771	0.000000
H	-1.574511	19.519771	0.000000
H	1.619895	20.336708	0.000000
H	-1.619895	-20.336708	0.000000
H	2.939954	-15.364110	-2.362975
H	-2.939954	15.364110	2.362975
H	2.939954	-15.364110	2.362975
H	-2.939954	15.364110	-2.362975
H	-2.674482	-16.576605	-2.524449
H	2.674482	16.576605	2.524449
H	-2.674482	-16.576605	2.524449
H	2.674482	16.576605	-2.524449
H	0.674411	-13.721419	-4.079357
H	-0.674411	13.721419	4.079357
H	0.674411	-13.721419	4.079357
H	-0.674411	13.721419	-4.079357
H	-0.286954	-18.265933	-4.054361
H	0.286954	18.265933	4.054361
H	-0.286954	-18.265933	4.054361
H	0.286954	18.265933	-4.054361

Table S5. RHF/6-31G* optimised Cartesian coordinates of **1(5)**.

Atom	X	Y	Z
C	0.381853	-1.199707	0.000000
C	-0.381853	1.199707	0.000000
C	-0.857105	2.775199	2.347260
C	0.857105	-2.775199	-2.347260
C	-0.857105	2.775199	-2.347260
C	0.857105	-2.775199	2.347260
C	0.734846	5.215229	2.348125
C	-0.734846	-5.215229	-2.348125
C	0.734846	5.215229	-2.348125
C	-0.734846	-5.215229	2.348125
C	0.265388	6.791549	0.000000
C	-0.265388	-6.791549	0.000000
C	-0.485506	9.195056	0.000000
C	0.485506	-9.195056	0.000000
C	-0.944445	10.775870	2.346885
C	0.944445	-10.775870	-2.346885
C	-0.944445	10.775870	-2.346885
C	0.944445	-10.775870	2.346885
C	0.678055	13.195865	2.348026
C	-0.678055	-13.195865	-2.348026
C	0.678055	13.195865	-2.348026
C	-0.678055	-13.195865	2.348026
C	0.226584	14.778037	0.000000
C	-0.226584	-14.778037	0.000000
C	-0.493131	17.191273	0.000000
C	0.493131	-17.191273	0.000000
C	-0.935069	18.775241	-2.355026
C	0.935069	-18.775241	2.355026
C	-0.935069	18.775241	2.355026
C	0.935069	-18.775241	-2.355026
C	0.765370	21.129024	2.382972
C	-0.765370	-21.129024	-2.382972
C	0.765370	21.129024	-2.382972
C	-0.765370	-21.129024	2.382972
C	0.411231	22.724995	0.000000
C	-0.411231	-22.724995	0.000000
H	-2.846046	3.305031	2.392550
H	2.846046	-3.305031	-2.392550
H	-2.846046	3.305031	-2.392550
H	2.846046	-3.305031	2.392550
H	2.723540	4.684624	2.397356
H	-2.723540	-4.684624	-2.397356
H	2.723540	4.684624	-2.397356
H	-2.723540	-4.684624	2.397356
H	-2.926453	11.331385	2.388916
H	2.926453	-11.331385	-2.388916
H	-2.926453	11.331385	-2.388916
H	2.926453	-11.331385	2.388916
H	2.660153	12.641380	2.396451
H	-2.660153	-12.641380	-2.396451
H	2.660153	12.641380	-2.396451

H	-2.660153	-12.641380	2.396451
H	-0.485019	1.751289	4.072333
H	0.485019	-1.751289	-4.072333
H	-0.485019	1.751289	-4.072333
H	0.485019	-1.751289	4.072333
H	0.359985	6.239706	4.072234
H	-0.359985	-6.239706	-4.072234
H	0.359985	6.239706	-4.072234
H	-0.359985	-6.239706	4.072234
H	-0.588676	9.747495	4.072731
H	0.588676	-9.747495	-4.072731
H	-0.588676	9.747495	-4.072731
H	0.588676	-9.747495	4.072731
H	0.317313	14.224921	4.072340
H	-0.317313	-14.224921	-4.072340
H	0.317313	14.224921	-4.072340
H	-0.317313	-14.224921	4.072340
H	2.901331	-19.391495	2.362366
H	-2.901331	19.391495	-2.362366
H	2.901331	-19.391495	-2.362366
H	-2.901331	19.391495	2.362366
H	0.656756	-17.720947	4.079214
H	-0.656756	17.720947	-4.079214
H	0.656756	-17.720947	-4.079214
H	-0.656756	17.720947	4.079214
H	-0.363519	-22.252435	4.054953
H	0.363519	22.252435	-4.054953
H	-0.363519	-22.252435	-4.054953
H	0.363519	22.252435	4.054953
H	-2.728032	-20.532415	2.523678
H	2.728032	20.532415	-2.523678
H	-2.728032	-20.532415	-2.523678
H	2.728032	20.532415	2.523678
H	1.482661	-23.530406	0.000000
H	-1.482661	23.530406	0.000000
H	-1.721673	-24.306257	0.000000
H	1.721673	24.306257	0.000000

Table S6. RHF/6-31G* optimised Cartesian coordinates of **2(1)**.

Atom	X	Y	Z
C	0.537486	-1.337269	2.637098
C	-0.537486	1.337269	-2.637098
C	0.537486	-1.337269	-2.637098
C	-0.537486	1.337269	2.637098
S	-0.537486	-3.253995	0.000000
S	0.537486	3.253995	0.000000
H	2.583118	-1.283675	2.660210
H	-2.583118	1.283675	-2.660210
H	2.583118	-1.283675	-2.660210
H	-2.583118	1.283675	2.660210
H	-0.086759	-2.332658	4.315390
H	0.086759	2.332658	-4.315390
H	-0.086759	-2.332658	-4.315390
H	0.086759	2.332658	4.315390

Table S7. RHF/6-31G* optimised Cartesian coordinates of **2(2)**.

Atom	X	Y	Z
C	-0.409226	-1.191850	0.000000
C	0.409226	1.191850	0.000000
C	0.907269	2.743111	2.365125
C	-0.907269	-2.743111	-2.365125
C	0.907269	2.743111	-2.365125
C	-0.907269	-2.743111	2.365125
C	-0.907269	4.991133	2.599299
C	0.907269	-4.991133	-2.599299
C	-0.907269	4.991133	-2.599299
C	0.907269	-4.991133	2.599299
S	-0.633970	7.213267	0.000000
S	0.633970	-7.213267	0.000000
H	2.829992	3.461738	2.291368
H	-2.829992	-3.461738	-2.291368
H	2.829992	3.461738	-2.291368
H	-2.829992	-3.461738	2.291368
H	0.765895	1.631987	4.071156
H	-0.765895	-1.631987	-4.071156
H	0.765895	1.631987	-4.071156
H	-0.765895	-1.631987	4.071156
H	-2.840150	4.323777	2.729680
H	2.840150	-4.323777	-2.729680
H	-2.840150	4.323777	-2.729680
H	2.840150	-4.323777	2.729680
H	-0.501018	6.059289	4.298131
H	0.501018	-6.059289	-4.298131
H	-0.501018	6.059289	-4.298131
H	0.501018	-6.059289	4.298131

Table S8. RHF/6-31G* optimised Cartesian coordinates of **2(3)**.

Atom	x	y	z
C	0.753482	1.246365	2.345719
C	-0.753482	-1.246365	-2.345719
C	0.753482	1.246365	-2.345719
C	-0.753482	-1.246365	2.345719
C	-0.232040	-2.810348	0.000000
C	0.232040	2.810348	0.000000
C	0.578435	-5.195688	0.000000
C	-0.578435	5.195688	0.000000
C	1.065337	-6.746057	2.367948
C	-1.065337	6.746057	-2.367948
C	1.065337	-6.746057	-2.367948
C	-1.065337	6.746057	2.367948
C	-0.753482	-8.991316	2.599973
C	0.753482	8.991316	-2.599973
C	-0.753482	-8.991316	-2.599973
C	0.753482	8.991316	2.599973
S	-0.482726	-11.212214	0.000000
S	0.482726	11.212214	0.000000
H	2.759329	0.786106	2.389695
H	-2.759329	-0.786106	-2.389695
H	2.759329	0.786106	-2.389695
H	-2.759329	-0.786106	2.389695
H	2.987215	-7.469303	2.306613
H	-2.987215	7.469303	-2.306613
H	2.987215	-7.469303	-2.306613
H	-2.987215	7.469303	2.306613
H	-2.685619	-8.321537	2.729000
H	2.685619	8.321537	-2.729000
H	-2.685619	-8.321537	-2.729000
H	2.685619	8.321537	2.729000
H	0.350857	2.251829	4.074122
H	-0.350857	-2.251829	-4.074122
H	0.350857	2.251829	-4.074122
H	-0.350857	-2.251829	4.074122
H	0.911889	-5.630266	4.070049
H	-0.911889	5.630266	-4.070049
H	0.911889	-5.630266	-4.070049
H	-0.911889	5.630266	4.070049
H	-0.350891	-10.062659	4.297756
H	0.350891	10.062659	-4.297756
H	-0.350891	-10.062659	-4.297756
H	0.350891	10.062659	4.297756

Table S9. RHF/6-31G* optimised Cartesian coordinates of **2(4)**.

Atom	X	Y	Z
C	-0.004555	-1.258938	0.000000
C	0.004555	1.258938	0.000000
C	0.027289	2.902344	2.348713
C	-0.027289	-2.902344	-2.348713
C	0.027289	2.902344	-2.348713
C	-0.027289	-2.902344	2.348713
C	2.271210	4.760356	2.344493
C	-2.271210	-4.760356	-2.344493
C	2.271210	4.760356	-2.344493
C	-2.271210	-4.760356	2.344493
C	2.276123	6.410550	0.000000
C	-2.276123	-6.410550	0.000000
C	2.255158	8.929705	0.000000
C	-2.255158	-8.929705	0.000000
C	2.271210	10.555002	2.368213
C	-2.271210	-10.555002	-2.368213
C	2.271210	10.555002	-2.368213
C	-2.271210	-10.555002	2.368213
C	4.689344	12.137750	2.598291
C	-4.689344	-12.137750	-2.598291
C	4.689344	12.137750	-2.598291
C	-4.689344	-12.137750	2.598291
S	5.105652	14.338347	0.000000
S	-5.105652	-14.338347	0.000000
H	-1.714790	3.998006	2.402647
H	1.714790	-3.998006	-2.402647
H	-1.714790	3.998006	-2.402647
H	1.714790	-3.998006	2.402647
H	4.014286	3.666218	2.375752
H	-4.014286	-3.666218	-2.375752
H	4.014286	3.666218	-2.375752
H	-4.014286	-3.666218	2.375752
H	0.662669	11.831744	2.309380
H	-0.662669	-11.831744	-2.309380
H	0.662669	11.831744	-2.309380
H	-0.662669	-11.831744	2.309380
H	6.325250	10.910224	2.722270
H	-6.325250	-10.910224	-2.722270
H	6.325250	10.910224	-2.722270
H	-6.325250	-10.910224	2.722270
H	0.086904	1.813002	4.072402
H	-0.086904	-1.813002	-4.072402
H	0.086904	1.813002	-4.072402
H	-0.086904	-1.813002	4.072402
H	2.232181	5.840157	4.074753
H	-2.232181	-5.840157	-4.074753
H	2.232181	5.840157	-4.074753
H	-2.232181	-5.840157	4.074753
H	2.078709	9.445731	4.070582
H	-2.078709	-9.445731	-4.070582
H	2.078709	9.445731	-4.070582

H	-2.078709	-9.445731	4.070582
H	4.635721	13.278065	4.298073
H	-4.635721	-13.278065	-4.298073
H	4.635721	13.278065	-4.298073
H	-4.635721	-13.278065	4.298073

Table S10. RHF/6-31G* optimised Cartesian coordinates of **2(5)**.

Atom	X	Y	Z
C	-0.796329	-1.219840	2.347566
C	0.796329	1.219840	-2.347566
C	-0.796329	-1.219840	-2.347566
C	0.796329	1.219840	2.347566
C	0.322293	2.794997	0.000000
C	-0.322293	-2.794997	0.000000
C	-0.440598	5.194522	0.000000
C	0.440598	-5.194522	0.000000
C	-0.922109	6.765147	2.349387
C	0.922109	-6.765147	-2.349387
C	-0.922109	6.765147	-2.349387
C	0.922109	-6.765147	2.349387
C	0.642732	9.222441	2.344700
C	-0.642732	-9.222441	-2.344700
C	0.642732	9.222441	-2.344700
C	-0.642732	-9.222441	2.344700
C	0.140178	10.793847	0.000000
C	-0.140178	-10.793847	0.000000
C	0.655178	-13.184229	0.000000
C	-0.655178	13.184229	0.000000
C	-1.139590	14.736213	2.367696
C	1.139590	-14.736213	-2.367696
C	-1.139590	14.736213	-2.367696
C	1.139590	-14.736213	2.367696
C	0.678237	16.982704	2.598602
C	-0.678237	-16.982704	-2.598602
C	0.678237	16.982704	-2.598602
C	-0.678237	-16.982704	2.598602
S	0.403152	19.204905	0.000000
S	-0.403152	-19.204905	0.000000
H	-2.785055	-0.689762	2.393600
H	2.785055	0.689762	-2.393600
H	-2.785055	-0.689762	-2.393600
H	2.785055	0.689762	2.393600
H	-2.916491	7.272879	2.405502
H	2.916491	-7.272879	-2.405502
H	-2.916491	7.272879	-2.405502
H	2.916491	-7.272879	2.405502
H	2.637624	8.716658	2.375597
H	-2.637624	-8.716658	-2.375597
H	2.637624	8.716658	-2.375597
H	-2.637624	-8.716658	2.375597
H	-0.423455	-2.243080	4.072686
H	0.423455	2.243080	-4.072686
H	-0.423455	-2.243080	-4.072686
H	0.423455	2.243080	4.072686
H	-0.528952	5.745821	4.072057
H	0.528952	-5.745821	-4.072057
H	-0.528952	5.745821	-4.072057
H	0.528952	-5.745821	4.072057
H	0.274032	10.238957	4.074547

H	-0.274032	-10.238957	-4.074547
H	0.274032	10.238957	-4.074547
H	-0.274032	-10.238957	4.074547
H	3.061699	-15.459405	-2.306977
H	-3.061699	15.459405	2.306977
H	3.061699	-15.459405	2.306977
H	-3.061699	15.459405	-2.306977
H	-2.610933	-16.313603	-2.723124
H	2.610933	16.313603	2.723124
H	-2.610933	-16.313603	2.723124
H	2.610933	16.313603	-2.723124
H	0.985517	-13.621731	-4.070616
H	-0.985517	13.621731	4.070616
H	0.985517	-13.621731	4.070616
H	-0.985517	13.621731	-4.070616
H	-0.278590	-18.052068	-4.298406
H	0.278590	18.052068	4.298406
H	-0.278590	-18.052068	4.298406
H	0.278590	18.052068	-4.298406