Supplementary Information

Cluster-in-molecule Approach with Explicitly Correlated Methods for Large Molecules

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1. Table S1 Benchmark calculations of CIM-MP2-F12 and CIM-DLPNO-F12 methods. The F12 correlation energies (in a.u.) are given.

	Natom	MP2-F12		DLPNO-CCSD-F12	
		CIM	Ref	CIM	ref
1	63	-1.01755	-1.01631	-0.73368	-0.73337
2	126	-1.44210	-1.44033	-1.46673	-1.46647
3	62	-0.68655	-0.68580	-0.48656	-0.48660

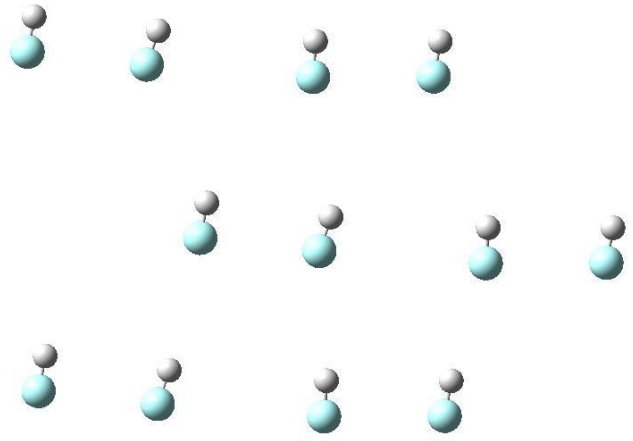
4	77	-1.12106	-1.11548	-0.80453	-0.80357
5	145	-2.37040	-2.37069	-1.71730	-1.71680
6	125	-2.19315	-2.18789	-1.48912	-1.48785

2. Table S2. Wall Times (in seconds) of various steps of the CIM-DLPNO-CCSD-F12 evaluation in the largest cluster

	2	4	6
Number of AOs (OBS/DF/CABS)	1377/3337/4854	903/2205/3201	1506/4054/5452
Cluster construction	76	17	123
Integral transformation	8027	1703	1840
DLPNO-CCSD iteration	3762	1209	754
Evaluation of C, V, X, B	12979	1903	5700
Total F12	15062	2521	7840
Total wall time	28437	5804	11504

3. Benchmark example of CIM-CCSD-F12

Geometry:



Coordiates:

F 0.83977046 -0.54255951 5.27132507

H	-0.04022954	-0.54255951	5.27132507
F	0.50079861	0.29492861	2.47005549
H	-0.37011224	0.28713641	2.34414454
F	-0.03302478	1.10323493	-1.46118695
H	-0.90706263	1.07861218	-1.36193189
F	-0.53094009	1.16138186	-4.33090307
H	-1.41094009	1.16138186	-4.33090307
F	4.38790418	0.88534292	0.48665624
H	3.50790418	0.88534292	0.48665624
F	4.04893233	1.72283104	-2.31461334
H	3.17802148	1.71503884	-2.44052429
F	3.51510894	2.53113736	-6.24585578
H	2.64107109	2.50651461	-6.14660072
F	3.01719363	2.58928429	-9.11557190
H	2.13719363	2.58928429	-9.11557190
F	8.49054776	2.06707791	3.80439088
H	7.61054776	2.06707791	3.80439088
F	8.15157591	2.90456603	1.00312130
H	7.28066506	2.89677383	0.87721035
F	7.61775252	3.71287235	-2.92812114
H	6.74371467	3.68824960	-2.82886608
F	7.11983721	3.77101928	-5.79783726
H	6.23983721	3.77101928	-5.79783726

Basis set: [cc-pVDZ-F12, aug-cc-pVDZ/C, cc-pVDZ-F12-OptRI]

Parameters: ξ = 3.5Å

Table S3 Benchmark calculations of CIM-CCSD-F12. CCSD and F12 energies are compared to the canonical values. Basis set employed is [cc-pVDZ-F12, cc-pVDZ-F12-OptRI, aug-cc-pVDZ-F12].

	CCSD	F12
CIM	-2.99155	-0.60702
Ref	-2.99241	-0.60748
Accuracy	99.97%	99.92%

4. Coordinates of benchmark examples (in Angstrom)

Sys 1.

c	-4.90006100	2.45629600	0.26716200
c	-5.14118500	1.02660300	0.23515900
n	-4.07194100	0.28283900	-0.25637700
c	-2.87588200	0.76414100	-0.71827300

n	-2.72886100	2.13717500	-0.68317600
c	-3.73036100	2.93689500	-0.19061600
o	-6.16411300	0.46925900	0.58891600
o	-1.99322100	0.03126600	-1.13320600
c	-1.48400200	2.70890200	-1.21570100
c	-0.25156700	2.33432500	-0.39906000
c	0.84843500	3.37088500	-0.60373400
n	2.10374800	2.83272200	-0.60735200
c	3.33217000	3.50702900	-0.62692400
o	0.59118500	4.55254900	-0.70297500
n	4.38565300	2.70597700	-0.42307600
c	5.61318500	3.24418700	-0.41003600
c	5.83767700	4.60942700	-0.62012900
c	4.72831500	5.40835300	-0.83227200
c	3.44526500	4.87897600	-0.83753900
n	6.63314800	2.33389900	-0.15142200
c	7.99640000	2.55913800	-0.16359200
o	8.50624200	3.62235000	-0.43396200
c	8.80145000	1.32170600	0.19323800
c	10.29822900	1.59398100	0.22210200
c	11.10421900	0.34717100	0.57639100
c	12.60854400	0.60530600	0.61191000
c	13.42144800	-0.63698500	0.96838600
c	14.92595300	-0.37929100	1.00398800
c	15.73674800	-1.62240000	1.36149800
c	17.24655100	-1.35946900	1.38870700
c	18.02910600	-2.57863800	1.77827300
c	18.91488600	-3.19175500	1.00374600
h	-5.67521000	3.10267900	0.64722300
h	-4.18623200	-0.74515200	-0.29853700
h	-3.50760600	3.99649100	-0.19785200
h	-1.59874100	3.79193000	-1.20944300
h	-1.36854300	2.37358500	-2.24752600
h	0.08861100	1.32839400	-0.63940200
h	-0.50092200	2.36541300	0.66727600
h	2.15823300	1.81795900	-0.65271700
h	6.84148700	4.99915900	-0.60973300
h	4.86438000	6.47090100	-0.99641600
h	2.56649100	5.48064400	-0.99761900
h	6.34469400	1.39562100	0.12026200
h	8.55755900	0.53500700	-0.52936400
h	8.44741700	0.94311700	1.15809100
h	10.50565900	2.39043500	0.94280800
h	10.61337300	1.98045700	-0.75133300

h	10.89026500	-0.44599900	-0.15031600
h	10.77910100	-0.03419800	1.55193200
h	12.82194400	1.39953000	1.33710200
h	12.93359300	0.98464000	-0.36412700
h	13.20739500	-1.43120800	0.24312300
h	13.09555900	-1.01548800	1.94475500
h	15.14106200	0.41512000	1.72875200
h	15.25226600	-0.00196600	0.02745000
h	15.52770600	-2.42046500	0.64084300
h	15.41627100	-1.99699500	2.34082600
h	17.44966000	-0.55167700	2.10214900
h	17.57811400	-1.00888200	0.40614500
h	17.82095800	-2.98215400	2.76807000
h	19.44072600	-4.08018300	1.33235800
h	19.14553200	-2.81931400	0.01037200

Sys 2.

C	4.90011200	-2.45613900	0.26795800
C	5.14122000	-1.02644800	0.23590800
N	4.07200600	-0.28273000	-0.25575400
C	2.87598200	-0.76405700	-0.71772200
N	2.72895200	-2.13709100	-0.68251100
C	3.73044200	-2.93677000	-0.18986800
O	6.16411800	-0.46905800	0.58969200
O	1.99337700	-0.03120300	-1.13279600
C	1.48420300	-2.70887400	-1.21523500
C	0.25154400	-2.33402800	-0.39906100
C	-0.84841300	-3.37064700	-0.60369200
N	-2.10372700	-2.83247900	-0.60759600
C	-3.33213100	-3.50681500	-0.62715700
O	-0.59115700	-4.55233600	-0.70261200
N	-4.38565200	-2.70579800	-0.42334400
C	-5.61316300	-3.24405600	-0.41031500
C	-5.83760800	-4.60930700	-0.62037000
C	-4.72821400	-5.40819500	-0.83248700
C	-3.44518600	-4.87877100	-0.83775400
N	-6.63315900	-2.33379400	-0.15173300
C	-7.99639800	-2.55906900	-0.16393400
O	-8.50620600	-3.62231700	-0.43423800
C	-8.80149700	-1.32166400	0.19288700
C	-10.29826100	-1.59401300	0.22181900
C	-11.10429400	-0.34725600	0.57619600
C	-12.60860200	-0.60547500	0.61180900
C	-13.42154900	0.63674900	0.96842100

C	-14.92603500	0.37896400	1.00413800
C	-15.73687400	1.62199500	1.36181400
C	-17.24665600	1.35896200	1.38916800
C	-18.02925300	2.57805000	1.77889800
C	-18.91519200	3.19113100	1.00452300
H	5.67524000	-3.10250400	0.64809500
H	4.18629400	0.74524500	-0.29798100
H	3.50770600	-3.99637000	-0.19706400
H	1.59887200	-3.79190800	-1.20865500
H	1.36906100	-2.37383900	-2.24719000
H	-0.08858300	-1.32818600	-0.63983200
H	0.50060000	-2.36473300	0.66735700
H	-2.15819600	-1.81771600	-0.65320700
H	-6.84140500	-4.99907300	-0.60998600
H	-4.86423500	-6.47075100	-0.99661400
H	-2.56639600	-5.48042300	-0.99779800
H	-6.34472100	-1.39548200	0.11984400
H	-8.55766500	-0.53497000	-0.52973700
H	-8.44745400	-0.94303900	1.15772400
H	-10.50561100	-2.39050300	0.94250800
H	-10.61343800	-1.98047200	-0.75161300
H	-10.89042800	0.44595000	-0.15049900
H	-10.77913300	0.03409800	1.55172800
H	-12.82190300	-1.39975300	1.33697000
H	-12.93370400	-0.98477000	-0.36422600
H	-13.20760400	1.43102600	0.24318500
H	-13.09560000	1.01521600	1.94478400
H	-15.14102900	-0.41551300	1.72886500
H	-15.25241500	0.00168800	0.02760300
H	-15.52796000	2.42012200	0.64119000
H	-15.41631800	1.99654700	2.34113200
H	-17.44963100	0.55111100	2.10258200
H	-17.57830300	1.00841200	0.40662100
H	-17.82100200	2.98153600	2.76868500
H	-19.44105900	4.07950000	1.33325000
H	-19.14594600	2.81871700	0.01116400
C	-4.90006100	2.45629600	0.26716200
C	-5.14118500	1.02660300	0.23515900
N	-4.07194100	0.28283900	-0.25637700
C	-2.87588200	0.76414100	-0.71827300
N	-2.72886100	2.13717500	-0.68317600
C	-3.73036100	2.93689500	-0.19061600
O	-6.16411300	0.46925900	0.58891600
O	-1.99322100	0.03126600	-1.13320600

C	-1.48400200	2.70890200	-1.21570100
C	-0.25156700	2.33432500	-0.39906000
C	0.84843500	3.37088500	-0.60373400
N	2.10374800	2.83272200	-0.60735200
C	3.33217000	3.50702900	-0.62692400
O	0.59118500	4.55254900	-0.70297500
N	4.38565300	2.70597700	-0.42307600
C	5.61318500	3.24418700	-0.41003600
C	5.83767700	4.60942700	-0.62012900
C	4.72831500	5.40835300	-0.83227200
C	3.44526500	4.87897600	-0.83753900
N	6.63314800	2.33389900	-0.15142200
C	7.99640000	2.55913800	-0.16359200
O	8.50624200	3.62235000	-0.43396200
C	8.80145000	1.32170600	0.19323800
C	10.29822900	1.59398100	0.22210200
C	11.10421900	0.34717100	0.57639100
C	12.60854400	0.60530600	0.61191000
C	13.42144800	-0.63698500	0.96838600
C	14.92595300	-0.37929100	1.00398800
C	15.73674800	-1.62240000	1.36149800
C	17.24655100	-1.35946900	1.38870700
C	18.02910600	-2.57863800	1.77827300
C	18.91488600	-3.19175500	1.00374600
H	-5.67521000	3.10267900	0.64722300
H	-4.18623200	-0.74515200	-0.29853700
H	-3.50760600	3.99649100	-0.19785200
H	-1.59874100	3.79193000	-1.20944300
H	-1.36854300	2.37358500	-2.24752600
H	0.08861100	1.32839400	-0.63940200
H	-0.50092200	2.36541300	0.66727600
H	2.15823300	1.81795900	-0.65271700
H	6.84148700	4.99915900	-0.60973300
H	4.86438000	6.47090100	-0.99641600
H	2.56649100	5.48064400	-0.99761900
H	6.34469400	1.39562100	0.12026200
H	8.55755900	0.53500700	-0.52936400
H	8.44741700	0.94311700	1.15809100
H	10.50565900	2.39043500	0.94280800
H	10.61337300	1.98045700	-0.75133300
H	10.89026500	-0.44599900	-0.15031600
H	10.77910100	-0.03419800	1.55193200
H	12.82194400	1.39953000	1.33710200
H	12.93359300	0.98464000	-0.36412700

H	13.20739500	-1.43120800	0.24312300
H	13.09555900	-1.01548800	1.94475500
H	15.14106200	0.41512000	1.72875200
H	15.25226600	-0.00196600	0.02745000
H	15.52770600	-2.42046500	0.64084300
H	15.41627100	-1.99699500	2.34082600
H	17.44966000	-0.55167700	2.10214900
H	17.57811400	-1.00888200	0.40614500
H	17.82095800	-2.98215400	2.76807000
H	19.44072600	-4.08018300	1.33235800
H	19.14553200	-2.81931400	0.01037200

Sys 3.

C	18.15854	-0.70215	-0.00307
C	16.80048	-1.38121	0.00051
C	15.58188	-0.44639	-0.00003
C	14.25454	-1.22168	0.00028
C	13.05338	-0.26337	0.00023
C	11.71251	-1.01252	-0.00013
C	10.52787	-0.03425	0.00004
C	9.17982	-0.76942	-0.00017
C	8.00000	0.21453	0.00009
C	6.65216	-0.52192	-0.00012
C	5.46955	0.45794	0.00011
C	4.12444	-0.28341	-0.00010
C	2.93933	0.69366	0.00012
C	1.59455	-0.04877	-0.00010
C	0.40827	0.92722	0.00012
C	-0.93685	0.18511	-0.00010
C	-2.12577	1.15869	0.00012
C	-3.46975	0.41351	-0.00010
C	-4.66324	1.38125	0.00012
C	-6.00151	0.63055	-0.00010
O	19.22658	-1.26563	-0.01751
O	18.08158	0.64084	0.01298
H	16.76002	-2.04330	-0.89647
H	16.76268	-2.03759	0.90170
H	15.61578	0.21014	0.90226
H	15.61630	0.20897	-0.90308
H	14.20491	-1.88007	-0.89931
H	14.20570	-1.88022	0.89983
H	13.10733	0.39466	0.90009
H	13.10733	0.39511	-0.89934
H	11.65277	-1.66951	-0.90012

H	11.65257	-1.66993	0.89953
H	10.59030	0.62301	0.89975
H	10.59037	0.62350	-0.89932
H	9.11521	-1.42592	-0.90019
H	9.11520	-1.42636	0.89953
H	8.06383	0.87163	0.90000
H	8.06386	0.87208	-0.89950
H	6.58932	-1.17880	-0.90013
H	6.58928	-1.17925	0.89957
H	5.53158	1.11480	0.90005
H	5.53162	1.11525	-0.89948
H	4.06325	-0.94062	-0.89999
H	4.06322	-0.94107	0.89945
H	3.00076	1.35075	0.90010
H	3.00080	1.35120	-0.89952
H	1.53463	-0.70610	-0.89993
H	1.53459	-0.70656	0.89940
H	0.46952	1.58426	0.90001
H	0.46956	1.58471	-0.89943
H	-0.99618	-0.47240	-0.89988
H	-0.99622	-0.47285	0.89934
H	-2.06589	1.81606	0.89997
H	-2.06585	1.81651	-0.89940
H	-3.52757	-0.24430	-0.89976
H	-3.52760	-0.24475	0.89922
H	-4.61014	2.03999	0.89981
H	-4.61010	2.04043	-0.89923
H	-6.85957	1.34154	0.00007
H	-6.09816	-0.01720	-0.90134
H	-6.09819	-0.01765	0.90081
H	18.98784	0.98924	0.01082

Sys 4.

F	8.0625	1.6775	1.8877
O	2.4595	-2.4468	0.0873
O	-9.8262	0.9092	1.7383
O	-7.8816	-0.9154	0.9265
N	6.9302	0.0351	-0.4119
N	-7.5284	1.0011	-0.3479
C	4.6374	-1.7786	-0.6319
C	4.7171	-0.6792	0.4326
C	5.5015	-1.3951	-1.8380
C	6.1692	-0.3492	0.7844
C	6.9278	-1.0421	-1.4107

C	8.3012	0.3967	-0.0521
C	8.4233	1.7999	0.5687
C	3.1921	-2.0326	-1.0510
C	-8.9285	1.4260	-0.4150
C	7.4737	2.8446	-0.0554
C	9.8622	2.3590	0.5510
C	-8.9348	2.4862	-1.5191
C	-7.5485	3.1115	-1.4141
C	-6.6622	1.9194	-1.0869
C	-9.4094	1.9877	0.9221
C	7.8045	3.2051	-1.4976
C	10.9042	1.4190	1.1431
C	-7.1370	-0.1562	0.3103
C	1.1237	-2.1301	0.1184
C	-5.7082	-0.4983	0.2774
C	0.4870	-1.9134	1.3405
C	0.4038	-2.0240	-1.0716
C	-4.8547	-0.0254	1.2743
C	-5.2056	-1.2959	-0.7507
C	-1.5895	-1.4845	0.1824
C	-2.9959	-1.1480	0.2149
C	-0.8695	-1.5907	1.3725
C	-0.9527	-1.7014	-1.0396
C	-3.4986	-0.3502	1.2430
C	-3.8494	-1.6206	-0.7819
H	5.0367	-2.7011	-0.1878
H	4.1948	-0.9906	1.3450
H	4.2152	0.2292	0.0737
H	5.0572	-0.5386	-2.3620
H	5.5322	-2.2247	-2.5544
H	6.6294	-1.2130	1.2823
H	6.1450	0.4689	1.5114
H	7.4757	-0.7238	-2.3061
H	7.4298	-1.9375	-1.0212
H	8.7394	-0.3577	0.6141
H	8.9125	0.4002	-0.9646
H	3.1554	-2.8260	-1.8068
H	2.7915	-1.1066	-1.4851
H	-9.5421	0.5624	-0.6988
H	7.5081	3.7593	0.5511
H	6.4318	2.5126	0.0136
H	10.1828	2.5858	-0.4708
H	9.8891	3.2953	1.1218
H	-9.7403	3.2202	-1.4263

H	-9.0357	1.9984	-2.4970
H	-7.2408	3.6251	-2.3290
H	-7.5270	3.8354	-0.5909
H	-6.3301	1.4077	-1.9968
H	-5.7871	2.1988	-0.4942
H	-10.2776	2.6393	0.7806
H	-8.6256	2.5475	1.4430
H	7.8735	2.3194	-2.1353
H	7.0138	3.8444	-1.9050
H	8.7380	3.7691	-1.5756
H	11.8783	1.9169	1.1851
H	11.0210	0.5155	0.5372
H	10.6318	1.1224	2.1607
H	-10.1325	1.2874	2.5801
H	1.0424	-2.0008	2.2704
H	0.8570	-2.2060	-2.0417
H	-5.2356	0.6026	2.0756
H	-5.8638	-1.6744	-1.5286
H	-1.3291	-1.4607	2.3484
H	-1.4661	-1.6053	-1.9924
H	-2.8672	0.0661	2.0231
H	-3.5099	-2.2694	-1.5845

Sys 5.

H	2.79600000	0.84000000	-0.71400000
C	2.76300000	1.90900000	-0.91900000
H	1.80600000	2.31400000	-0.59400000
H	2.89800000	2.08200000	-1.98400000
C	3.87700000	2.58700000	-0.15700000
O	4.63300000	1.93000000	0.54600000
N	3.97800000	3.90600000	-0.29700000
H	3.32100000	4.38900000	-0.89200000
C	4.99400000	4.72700000	0.36400000
H	4.91200000	4.60200000	1.44400000
H	5.98500000	4.39200000	0.05700000
C	4.85200000	6.21300000	0.02900000
O	3.96800000	6.60300000	-0.73400000
N	5.72300000	7.04700000	0.59900000
H	6.44400000	6.66600000	1.19800000
C	5.75300000	8.50500000	0.39300000
H	5.47000000	8.70500000	-0.64100000
C	4.71800000	9.20500000	1.30600000
H	3.75200000	8.72800000	1.14100000
C	5.04600000	9.08800000	2.80100000

H	5.98400000	9.59300000	3.03000000
H	4.24700000	9.54100000	3.38700000
H	5.12800000	8.03900000	3.08300000
C	4.54700000	10.69000000	0.96500000
H	4.34200000	10.80600000	-0.10000000
H	3.70100000	11.09300000	1.52300000
H	5.43800000	11.25900000	1.23200000
C	7.17700000	9.03700000	0.59500000
O	7.95800000	8.44900000	1.34000000
N	7.52200000	10.14100000	-0.07100000
H	6.83000000	10.59400000	-0.65100000
C	8.82700000	10.81500000	0.02700000
H	9.19500000	10.69400000	1.04600000
C	9.85200000	10.15300000	-0.92300000
H	9.86000000	9.08300000	-0.71300000
C	9.51000000	10.33300000	-2.40900000
H	9.53600000	11.38700000	-2.68400000
H	10.23200000	9.79000000	-3.01900000
H	8.51700000	9.93400000	-2.61400000
C	11.27900000	10.66400000	-0.69100000
H	11.53900000	10.57400000	0.36400000
H	11.97800000	10.06000000	-1.27000000
H	11.37900000	11.70300000	-1.00500000
C	8.65600000	12.31600000	-0.22900000
O	7.72900000	12.72500000	-0.92800000
N	9.53200000	13.14500000	0.34200000
H	10.30000000	12.75400000	0.87200000
C	9.54300000	14.60200000	0.16900000
H	9.20600000	14.83600000	-0.84200000
C	8.55300000	15.24000000	1.16300000
H	7.58700000	14.73800000	1.08400000
H	8.92300000	15.10100000	2.17900000
C	8.33200000	16.71100000	0.92100000
N	9.03400000	17.74300000	1.54200000
C	8.65500000	18.87200000	0.92800000
H	9.04000000	19.85600000	1.16200000
N	7.76400000	18.60100000	-0.04100000
H	7.36500000	19.28300000	-0.67000000
C	7.55300000	17.23900000	-0.06600000
H	6.93600000	16.68200000	-0.75800000
C	10.97200000	15.15600000	0.31100000
O	11.86900000	14.44700000	0.76700000
N	11.19100000	16.40700000	-0.09500000
H	10.39300000	16.96600000	-0.37100000

C	12.45600000	17.12400000	0.04700000
H	12.83700000	16.97700000	1.05800000
H	13.18500000	16.72800000	-0.65900000
C	12.28700000	18.62500000	-0.20500000
O	11.34900000	19.05200000	-0.87900000
N	13.19500000	19.43400000	0.34400000
H	13.95300000	19.02600000	0.87500000
C	13.19500000	20.90200000	0.23200000
H	12.85800000	21.16500000	-0.77100000
C	12.19800000	21.52000000	1.24100000
H	11.22900000	21.04400000	1.08800000
C	12.59500000	21.29800000	2.70700000
H	13.54100000	21.79300000	2.92800000
H	11.82200000	21.70200000	3.36200000
H	12.69400000	20.23200000	2.90900000
C	11.99100000	23.02400000	1.01900000
H	11.73900000	23.21400000	-0.02400000
H	11.16700000	23.37200000	1.64300000
H	12.88600000	23.58500000	1.28700000
C	14.61900000	21.44300000	0.40100000
O	15.44800000	20.81700000	1.06000000
N	14.91200000	22.59900000	-0.19500000
H	14.18800000	23.07900000	-0.71100000
C	16.21000000	23.28900000	-0.12700000
H	16.75100000	22.94900000	0.75600000
C	17.08200000	22.98300000	-1.36100000
H	18.02100000	23.53000000	-1.26500000
C	17.41700000	21.50200000	-1.52400000
H	16.51600000	20.93200000	-1.75100000
H	18.13500000	21.37400000	-2.33400000
H	17.85500000	21.12200000	-0.60100000
O	16.43900000	23.40200000	-2.54000000
H	17.02700000	23.22500000	-3.27700000
C	16.01000000	24.80100000	0.01500000
O	14.90400000	25.31400000	-0.15600000
N	17.07900000	25.52400000	0.35600000
H	17.96800000	25.06300000	0.48100000
C	17.09300000	26.98600000	0.53600000
H	16.27600000	27.42400000	-0.03800000
C	16.90000000	27.38000000	2.01400000
H	16.92400000	28.46700000	2.08700000
C	15.58200000	26.89900000	2.61800000
H	15.56900000	25.81200000	2.68800000
H	15.45600000	27.32400000	3.61300000

H	14.75200000	27.22400000	1.98900000
O	17.93900000	26.85600000	2.80500000
H	17.75400000	27.07800000	3.72100000
C	18.40000000	27.57900000	-0.00300000
O	19.34500000	26.85300000	-0.31100000
N	18.45300000	28.90700000	-0.14400000
H	17.65600000	29.46300000	0.13200000
C	19.62700000	29.65800000	-0.61900000
H	20.52200000	29.14400000	-0.26500000
C	19.67300000	29.66900000	-2.16500000
H	19.60300000	28.63700000	-2.50900000
C	18.51600000	30.45100000	-2.80200000
H	18.56500000	31.50500000	-2.52600000
H	18.57100000	30.36600000	-3.88800000
H	17.56200000	30.04000000	-2.47300000
C	20.99200000	30.23200000	-2.70800000
H	21.83400000	29.71300000	-2.24700000
H	21.03800000	30.06900000	-3.78500000
H	21.07100000	31.30200000	-2.51700000
C	19.62600000	31.06400000	-0.00900000
O	18.56700000	31.59000000	0.33200000
N	20.80400000	31.67100000	0.14200000
H	21.63700000	31.20700000	-0.19100000
C	20.99000000	33.02200000	0.67100000
H	20.12500000	33.63100000	0.40200000
C	21.07900000	32.94700000	2.20200000
H	21.93800000	32.34200000	2.49500000
H	21.18800000	33.94800000	2.62000000
H	20.17000000	32.49700000	2.60300000
C	22.24100000	33.68000000	0.05700000
O	23.10000000	32.99100000	-0.49200000
N	22.34400000	35.01200000	0.15800000
H	21.60300000	35.50900000	0.62700000
C	23.46800000	35.78600000	-0.36600000
H	23.54900000	35.63400000	-1.44400000
H	23.32500000	36.84800000	-0.16200000
H	24.39600000	35.45100000	0.10100000

Sys 6.

Si	1.45480300	-1.41577500	4.43711900
O	2.35782700	-5.08722100	1.90649800
H	6.16229400	4.99060800	-1.90380700
Si	0.84033200	-5.40399700	1.55406200
O	2.36041100	-5.09689600	-1.85841100

H	6.15967300	5.00043600	1.90508200
Si	0.84244000	-5.41189500	-1.50642600
O	-1.94778900	-3.56434500	4.14620500
H	0.58696700	-6.84364700	-1.72050800
Si	-0.38285700	-3.82495200	3.86935400
O	-1.94210100	-3.58565400	-4.11186600
H	0.58456000	-6.83462700	1.77517800
Si	-0.37755400	-3.84482200	-3.83151800
O	-3.75921300	4.02900600	-1.93786300
H	-3.55932700	-5.49099900	3.82796500
Si	1.38321600	1.56603400	-3.74943800
O	-5.43870000	4.51608700	-0.00616300
H	-3.55408300	-5.51064500	-3.78590600
Si	1.46083500	-1.43862200	-4.40916300
O	-4.46850800	-3.17409800	3.91266100
H	-3.42817200	-4.32779200	-5.87748000
Si	-3.35771700	-4.17481200	4.45081000
O	-4.46314000	-3.19421600	-3.88381100
H	-6.82780500	-4.03877000	-3.85395900
Si	-3.35161100	-4.19768800	-4.41525700
O	-5.98888500	2.80215800	1.86648500
H	-6.35725400	-1.88165400	-4.86660500
Si	-5.29609400	4.18398600	1.53696300
O	-5.98631100	2.79251600	-1.87059900
H	-8.56290100	-1.41178900	-1.84912500
Si	-5.29397800	4.17603200	-1.54729200
O	-6.21420100	-2.08770900	2.40225000
H	-7.19682900	1.83044300	-3.85385900
Si	-6.01493600	-2.79957800	3.81383000
O	-6.21090600	-2.10005300	-2.38143200
H	-8.43316800	2.27474900	-1.84664900
Si	-6.00970000	-2.81919500	-3.78904300
O	-6.80766000	0.37315000	1.89009000
H	-8.43570800	2.28426800	1.84183800
Si	-7.14196400	1.84505500	2.38426400
O	-6.80506200	0.36341300	-1.88279600
H	-7.20213600	1.85032900	3.85301500
Si	-7.13867900	1.83274900	-2.38501800
O	-6.83060300	-1.42691000	0.00821200
H	-8.56545700	-1.40220900	1.86316100
Si	-7.15736000	-1.12649000	1.54371800
O	4.93496700	3.91936200	0.00261900
H	-6.36397000	-1.85649000	4.88606000
Si	-7.15524300	-1.13441900	-1.52917100

O	5.27490100	0.83174100	3.76975300
H	-6.83313400	-4.01880400	3.88391200
Si	6.05929900	-0.36438500	4.44746300
O	5.28007800	0.81234200	-3.74813900
H	-3.43629200	-4.29736700	5.91357700
Si	6.06540500	-0.38726300	-4.41860600
O	4.79521600	2.93820100	2.36506700
H	0.07228000	-4.71221800	4.94946100
Si	4.92531900	4.28873900	1.54381000
O	4.79847300	2.92600800	-2.35502000
H	4.28427400	-3.71815100	4.89819700
Si	4.92742300	4.28077000	-1.54052400
O	5.46397500	-1.73836200	3.91579700
H	5.93532900	-0.27781100	5.90966000
Si	4.46202000	2.19313200	3.72829400
O	5.46934500	-1.75847900	-3.88067600
H	-5.92252100	5.26515900	-2.30863700
Si	4.46715300	2.17387800	-3.71481100
O	3.72415900	5.25103900	-1.87024600
H	-5.92569100	5.27702900	2.29184700
Si	4.21210800	-2.72083300	3.82066900
O	4.32754100	-3.45861100	2.41304800
H	5.94344900	-0.30823600	-5.88139800
Si	4.21734200	-2.74045100	-3.78220400
O	4.33079900	-3.47094100	-2.37063600
H	1.49980300	-1.39948400	-5.87814300
Si	2.27791300	5.64409300	-2.38860100
O	4.04326300	-4.32774800	0.02327500
H	4.29099000	-3.74331600	-4.85446900
Si	3.86869800	-4.72886100	1.56058900
O	0.73649900	2.11123000	-2.40132700
H	0.07906700	-4.73764900	-4.90640400
Si	3.87085300	-4.73690500	-1.51224000
O	1.11736100	0.02117600	3.81664800
H	4.86269000	3.04263100	4.85904800
Si	-2.37565100	4.68145700	-2.38502800
O	-3.76191300	4.03899300	1.93048800
H	2.22596900	5.61427600	-3.85713400
Si	0.29013900	3.36548300	-1.56396400
O	3.72151200	5.26066300	1.86675900
H	1.99477100	7.01190300	-1.93100500
Si	1.34937700	1.59478300	3.76706900
O	2.91874800	1.88829700	3.80303100
H	-2.27154100	4.76544400	-3.84884000

Si	2.24803700	5.71557000	2.36487000
O	1.20687600	4.63587400	-1.80426100
H	-2.27730500	6.03249300	-1.81419900
Si	-2.35911900	4.68794500	2.34765100
O	-1.21884600	3.73716100	-1.83587100
H	0.73080400	2.19776700	-4.90525000
O	1.12275300	0.00157800	-3.79661200
O	0.78942700	2.05028300	2.36943100
H	4.86937600	3.01757800	-4.84941500
O	0.33595000	-2.43321100	-3.89637000
O	0.56277300	2.69434800	-0.07454200
H	0.73660400	2.20838700	4.88435300
O	-0.10346700	-4.51577300	-2.41479400
O	-1.37707700	3.66875800	1.61926500
H	2.21931000	5.63380500	3.82016200
O	0.33057700	-2.41302900	3.92788100
O	1.12574300	4.85562600	1.62702200
H	-2.27786400	4.77922500	3.80085500
O	0.51620800	-5.04977600	0.02272100
H	1.49167300	-1.36908000	5.90591600
H	1.98935200	7.02572500	1.91240200
O	-0.10682000	-4.50320400	2.45648900
H	4.74380900	-5.86312400	1.89013400
H	-2.27991000	6.01593600	1.80474200
O	2.92404200	1.86887900	-3.79027800
H	4.74639400	-5.87271800	-1.83475500
H	0.70961400	1.72698500	-0.03946600
O	2.86167800	-1.88835800	3.89049800
H	7.50129600	-0.33867300	4.16308900
Al	0.26940300	3.41584600	1.55628700
O	2.86701100	-1.90835600	-3.85818100
H	7.50701000	-0.36007600	-4.13238200

5. Coordinates of extended and folded $C_{30}H_{62}$ (in Angstrom)

extended

C	5.790306	-0.404884	0.000326
H	5.792115	-1.067301	-0.879149
H	5.792197	-1.067208	0.879869
C	4.501484	0.433644	0.000339
H	4.499608	1.095984	-0.879193
H	4.499665	1.096046	0.879824
C	3.217357	-0.412059	0.000408
H	3.219228	-1.074400	0.879939
H	3.219178	-1.074459	-0.879079

C	1.928538	0.426475	0.000414
H	1.926682	1.088833	-0.879104
H	1.926706	1.088859	0.879913
C	0.644409	-0.419224	0.000441
H	0.646248	-1.081607	-0.879059
H	0.646260	-1.081582	0.879959
C	-0.644410	0.419310	0.000435
H	-0.646243	1.081690	-0.879068
H	-0.646267	1.081672	0.879949
C	-1.928537	-0.426391	0.000404
H	-1.926707	-1.088773	0.879905
H	-1.926674	-1.088751	-0.879113
C	-3.217359	0.412138	0.000390
H	-3.219180	1.074534	-0.879099
H	-3.219236	1.074482	0.879918
C	-4.501480	-0.433573	0.000320
H	-4.499660	-1.095972	0.879807
H	-4.499598	-1.095915	-0.879210
C	-5.790309	0.404946	0.000301
H	-5.792123	1.067359	-0.879176
H	-5.792207	1.067272	0.879842
C	-7.074420	-0.440780	0.000194
H	-7.072607	-1.103195	0.879669
H	-7.072517	-1.103104	-0.879349
C	-8.363256	0.397727	0.000171
H	-8.365068	1.060152	-0.879295
H	-8.365176	1.060037	0.879724
C	-9.647354	-0.448021	0.000035
H	-9.645543	-1.110447	0.879500
H	-9.645432	-1.110328	-0.879520
C	-10.936196	0.390479	0.000009
H	-10.938005	1.052911	-0.879451
H	-10.938131	1.052773	0.879571
C	-12.220275	-0.455301	-0.000151
H	-12.218468	-1.117727	0.879311
H	-12.218339	-1.117587	-0.879718
C	7.074425	0.440830	0.000218
H	7.072618	1.103247	0.879692
H	7.072529	1.103152	-0.879327
C	8.363252	-0.397692	0.000197
H	8.365164	-1.059998	0.879752
H	8.365054	-1.060120	-0.879267
C	9.647360	0.448040	0.000055
H	9.645561	1.110468	0.879519

H	9.645444	1.110345	-0.879501
C	10.936190	-0.390479	0.000026
H	10.937985	-1.052913	-0.879431
H	10.938118	-1.052771	0.879591
C	12.220282	0.455280	-0.000141
H	12.218353	1.117565	-0.879710
H	12.218491	1.117709	0.879319
C	13.509093	-0.383276	-0.000174
H	13.510874	-1.045700	-0.879626
H	13.511023	-1.045542	0.879395
C	14.793205	0.462526	-0.000360
H	14.791323	1.124942	0.879134
H	14.791172	1.124784	-0.879972
C	16.081982	-0.375837	-0.000396
H	16.084589	-1.038507	-0.879886
H	16.084747	-1.038341	0.879220
C	17.367111	0.469250	-0.000591
H	17.363681	1.130606	-0.879835
H	17.363839	1.130773	0.878529
C	18.649231	-0.379085	-0.000626
H	18.693523	-1.026863	-0.886211
H	19.548402	0.249387	-0.000767
H	18.693683	-1.026694	0.885074
C	-13.509100	0.383233	-0.000179
H	-13.510898	1.045655	-0.879632
H	-13.511037	1.045502	0.879389
C	-14.793197	-0.462591	-0.000355
H	-14.791298	-1.125006	0.879140
H	-14.791158	-1.124851	-0.879966
C	-16.081989	0.375748	-0.000384
H	-16.084615	1.038416	-0.879877
H	-16.084760	1.038254	0.879230
C	-17.367103	-0.469363	-0.000569
H	-17.363812	-1.130884	0.878552
H	-17.363666	-1.130721	-0.879811
C	-18.649239	0.378948	-0.000597
H	-18.693549	1.026722	-0.886183
H	-19.548397	-0.249542	-0.000729
H	-18.693697	1.026558	0.885102

folded

C	3.95146500	-1.93345900	0.33599900
H	3.93709500	-0.99166200	0.90415700
H	3.99242000	-2.73921700	1.08463400

C	5.21989800	-1.96721900	-0.53283200
H	5.30158200	-2.94069500	-1.03984000
H	5.11832700	-1.21779700	-1.33258700
C	6.50579900	-1.67144500	0.25635100
H	6.68292900	-2.46769200	0.99455300
H	6.34698200	-0.75944300	0.84084100
C	7.76049500	-1.51484200	-0.63005400
H	7.49297800	-0.98844900	-1.55791300
H	8.09334200	-2.51443200	-0.94328800
C	8.93900500	-0.77336700	0.04693900
H	9.87893500	-1.12353000	-0.40224500
H	8.98543100	-1.06618100	1.10737500
C	8.93891900	0.77319100	-0.04779400
H	8.98499900	1.06596500	-1.10825400
H	9.87896100	1.12339700	0.40111700
C	7.76050000	1.51447700	0.62956800
H	8.09337600	2.51399100	0.94301400
H	7.49313700	0.98784800	1.55733400
C	6.50565700	1.67133300	-0.25658900
H	6.34673100	0.75948100	-0.84130300
H	6.68268000	2.46776900	-0.99461300
C	5.21990300	1.96694700	0.53289200
H	5.30186800	2.94016500	1.04035600
H	5.11829900	1.21718300	1.33232100
C	3.95131400	1.93387800	-0.33574000
H	3.93659400	0.99229400	-0.90425300
H	3.99236900	2.73989500	-1.08408700
C	2.64806500	2.04532000	0.47130700
H	2.63408600	2.99944500	1.02014600
H	2.63291500	1.25413600	1.23644900
C	1.38095000	1.93303200	-0.39163300
H	1.40784400	0.98539300	-0.94963100
H	1.38300600	2.73230700	-1.14862100
C	0.07765800	2.00489500	0.41978300
H	0.05338900	2.94888700	0.98577100
H	0.07445800	1.20044200	1.17069200
C	-1.19070100	1.89870600	-0.44184600
H	-1.16914000	0.95420700	-1.00482000
H	-1.18578800	2.70199000	-1.19463300
C	-2.49248200	1.97507300	0.37166300
H	-2.50717700	2.91496700	0.94477300
H	-2.50248000	1.16529900	1.11641400
C	-3.76284700	1.88775400	-0.48911800
H	-3.74954300	0.94907900	-1.06192900

H	-3.75275200	2.69864500	-1.23364100
C	-5.06293000	1.96509800	0.32710800
H	-5.07327300	2.90205700	0.90511100
H	-5.07428500	1.15154000	1.06756700
C	-6.33507800	1.88563800	-0.53165500
H	-6.32266600	0.95236100	-1.11371500
H	-6.32819300	2.70349800	-1.26879900
C	-7.63455200	1.95308300	0.28752500
H	-7.64728100	2.88782400	0.86749200
H	-7.63703200	1.13777500	1.02487400
C	2.64807900	-2.04487200	-0.47080100
H	2.63290700	-1.25378900	-1.23605300
H	2.63397900	-2.99905300	-1.01954800
C	1.38102500	-1.93240100	0.39216700
H	1.38317100	-2.73136500	1.14948300
H	1.40786100	-0.98453200	0.94977500
C	0.07774000	-2.00468300	-0.41919500
H	0.07430800	-1.20032300	-1.17020500
H	0.05376100	-2.94874500	-0.98508200
C	-1.19065000	-1.89877200	0.44239500
H	-1.18576000	-2.70226100	1.19496300
H	-1.16917000	-0.95442900	1.00563900
C	-2.49233400	-1.97502600	-0.37126800
H	-2.50692100	-2.91484900	-0.94449900
H	-2.50225200	-1.16516200	-1.11591700
C	-3.76281600	-1.88788000	0.48934700
H	-3.74961200	-0.94932600	1.06236500
H	-3.75282300	-2.69893900	1.23368800
C	-5.06275700	-1.96515600	-0.32711400
H	-5.07296100	-2.90209500	-0.90515400
H	-5.07399900	-1.15157400	-1.06754500
C	-6.33506500	-1.88580000	0.53142000
H	-6.32277200	-0.95259300	1.11359800
H	-6.32831300	-2.70375200	1.26846300
C	-7.63439400	-1.95320800	-0.28800300
H	-7.64700100	-2.88792200	-0.86801700
H	-7.63678500	-1.13787000	-1.02531600
C	-8.90207400	-1.86737100	0.57651200
H	-8.92870400	-0.92950800	1.14552600
H	-9.81090200	-1.91067700	-0.03607100
H	-8.94394400	-2.69418800	1.29778500
C	-8.90208000	1.86716300	-0.57720400
H	-8.92859000	0.92926100	-1.14615900
H	-9.81101500	1.91049000	0.03521800

H -8.94384000 2.69393100 -1.29853900

5. Comparison between DLPNO-CCSD(T0) and (T1)

5.1. Alkane $C_{32}H_{64}$

Table S4. Relative energies (kcal/mol) between the extended and folded conformers, with the cc-pVDZ-F12 basis set

	extended	folded	ΔE
T0	-0.19996	-0.20406	-2.57
T1	-0.20615	-0.21045	-2.70

5.2 Polyglycine

Table S5. Relative energies among the C5, C7 and C10 conformers of polyglycine, with the cc-pVDZ-F12 basis set, in the parenthesis is the relative energies (kcal/mol) to the C5 conformer

	C5	C7	C10
T0	-0.33157(0.)	-0.33634(-2.99)	-0.33514(-2.24)
T1	-0.34869(0.)	-0.35391(-3.27)	-0.35236(-2.30)

6. Table S6. Comparison of CIM and canonical MP2 correlation energies (a.u.) of the S30L-23 system

	AB	A	B
CIM-RI-MP2	-8.73515	-5.22887	-3.47931
RI-MP2	-8.73876	-5.22911	-3.47961
Accuracy	99.96%	99.99%	99.99%