Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

An efficient method for generating property-energy consistent basis sets. New pecJ-*n* (*n* = 1, 2) basis sets for high-quality calculations of indirect nuclear spin-spin coupling constants involving ^{1}H, ^{13}C, ^{15}N, and ^{19}F nuclei

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Supplementary Information

Basis sets are given CFOUR format

```
H:pecJ-1
Property-energy consistent basis set

 2
  0   1
  5   2
  7   2

5.07308E+03  2.16644E+02  2.50008E+01  5.00205E+00  1.29556E+00
4.00307E-01  1.33227E-01

 1.6152E-05  0.00000000  0.00000000  0.00000000  0.00000000
 5.6257E-04  0.00000000  0.00000000  0.00000000  0.00000000
 6.0071E-03  0.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  1.00000000  0.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  1.00000000  0.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  1.00000000  0.00000000
 0.00000000  0.00000000  0.00000000  0.00000000  1.00000000

 1.48544E+00  4.06750E-01

 1.00000000  0.00000000
 0.00000000  1.00000000


C:pecJ-1
Property-energy consistent basis set

 3
  0   1   2
  8   3   2
 10   5   2

3.551632E+04  5.744652E+03  9.954157E+02  2.315943E+02  6.620654E+01
2.157261E+01  7.648720E+00  2.844272E+00  6.482868E-01  2.179306E-01

 7.5298E-05  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
 6.8542E-04  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
 5.2333E-03  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
0.00000000  1.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
0.00000000
0.00000000  0.00000000  1.00000000  0.00000000  0.00000000  0.00000000  0.00000000
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1.00000000

3.053233E+01 6.903835E+00 1.882246E+00 5.969291E-01 1.734469E-01

4.2186E-03 0.00000000 0.00000000
3.2808E-02 0.00000000 0.00000000
1.1902E-01 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 1.00000000

1.234913E+00 3.853405E-01

1.00000000 0.00000000
0.00000000 1.00000000

N:pecJ-1
Property-energy consistent basis set

3
0 1 2
8 3 2
10 5 2

1.649023E+05 9.215658E+03 1.455967E+03 3.238329E+02 8.920075E+01
2.841262E+01 1.001470E+01 3.764414E+00 7.224090E-01 2.026552E-01

2.8965E-05 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
6.4303E-04 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
4.9523E-03 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
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0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
1.00000000

3.123160E+01 6.893201E+00 1.978571E+00 6.571405E-01 1.946419E-01

7.8950E-03 0.00000000 0.00000000
5.5666E-02 0.00000000 0.00000000
1.6792E-01 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 1.00000000

1.411561E+00 3.724804E-01

1.00000000 0.00000000
0.00000000 1.00000000

F:pecJ-1
Property-energy consistent basis set

3
0 1 2
8 3 2
10 5 2

2.282510E+05 1.395200E+04 2.238199E+03 5.097673E+02 1.430299E+02
4.604822E+01 1.633767E+01 6.221429E+00 1.267895E+00 3.612004E-01

3.5113E-05 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
7.1935E-04 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
5.3999E-03 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 1.00000000 0.00000000 0.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00000000 0.00000000
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0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
1.00000000

9.142507E+01 1.727983E+01 4.618007E+00 1.355099E+00 3.034276E-01

5.5622E-03 0.00000000 0.00000000
5.4380E-02 0.00000000 0.00000000
2.1629E-01 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 1.00000000

2.207200E+00 4.610628E-01

1.00000000 0.00000000
0.00000000 1.00000000

H:pecJ-2
Property-energy consistent basis set

3
0 1 2
6 3 1
8 3 1

3.26942E+04 3.09626E+03 1.76078E+02 2.25414E+01 4.68174E+00
1.25964E+00 3.88875E-01 1.26668E-01

6.8514E-07 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
2.6416E-05 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
6.8682E-04 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 1.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 1.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000

2.35117E+00 7.73294E-01 2.79310E-01

1.00000000 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 1.00000000

1.07027E+00

1.00000000

C:pecJ-2
Property-energy consistent basis set

4
0 1 2 3
9 4 3 1
11 6 3 1

1.620383E+05 8.803354E+03 1.333357E+03 3.008000E+02 8.511667E+01
2.752030E+01 9.731687E+00 3.570774E+00 8.102360E-01 3.593953E-01
1.356139E-01

2.0172E-05 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000
4.7447E-04 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000
3.7131E-03 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000
0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000
0.00000000 0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000
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0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
1.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 1.00000000

9.495948E+01 1.778687E+01 4.534333E+00 1.336460E+00 4.353544E-01
1.348775E-01

7.9297E-04 0.00000000 0.00000000 0.00000000
8.7271E-03 0.00000000 0.00000000 0.00000000
5.0608E-02 0.00000000 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000 0.00000000

0.00000000 0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 0.00000000 1.00000000

6.136738E+00 1.157001E+00 3.542131E-01

1.00000000 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 1.00000000

7.838496E-01

1.00000000

N:pecJ-2
Property-energy consistent basis set

4
0 1 2 3
9 4 3 1
11 6 3 1

2.079517E+05 1.292159E+04 1.817985E+03 4.082074E+02 1.167577E+02
3.805405E+01 1.337707E+01 4.904271E+00 1.419406E+00 5.160150E-01
1.537757E-01

2.0018E-05 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000
4.4894E-04 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000
3.8478E-03 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000
0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000
0.00000000 0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000
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0.00000000 0.00000000 0.00000000 1.00000000 0.00000000 0.00000000 0.00000000
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0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
1.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 1.00000000

5.465743E+01 1.370955E+01 4.095889E+00 1.373762E+00 4.870015E-01
1.595081E-01

3.0587E-03 0.00000000 0.00000000 0.00000000
2.0245E-02 0.00000000 0.00000000 0.00000000
8.5787E-02 0.00000000 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000 0.00000000
0.00000000 0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 0.00000000 1.00000000

4.573625E+00 1.031398E+00 2.690828E-01

1.00000000 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 1.00000000

1.051532E+00

1.00000000

F:pecJ-2
Property-energy consistent basis set

4
0 1 2 3
9 4 3 1
11 6 3 1

3.22435E+05 1.95000E+04 2.92300E+03 6.64500E+02 1.87500E+02
6.06200E+01 2.14200E+01 7.95000E+00 2.25700E+00 8.81500E-01
3.04100E-01

2.2532E-05 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000
4.9256E-04 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000
3.9372E-03 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000
0.00000000 1.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
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1.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 1.00000000

2.84686E+02 4.38800E+01 9.92600E+00 2.93000E+00 9.13200E-01
2.67200E-01

9.2165E-04 0.00000000 0.00000000 0.00000000
1.5560E-02 0.00000000 0.00000000 0.00000000
1.0143E-01 0.00000000 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000 0.00000000
0.00000000 0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 0.00000000 1.00000000

4.10694E+00 1.19313E+00 1.98893E-01

1.00000000 0.00000000 0.00000000
0.00000000 1.00000000 0.00000000
0.00000000 0.00000000 1.00000000

1.89198E+00

1.00000000

Table S1. The SSCCs (in Hz) calculated at the CCSD level (J_{CCSD}) with taking into account solvent (Δ_{solv}) and vibrational (Δ_{vib}) corrections using the pecJ-*n* (*n* = 1, 2), ccJ-pVXZ (X=D, T), and pcJ-*n* (*n* = 1,2) basis sets.

Molecule	SSCC	Basis set	N_{bas}	J_{CCSD}	Δ_{vib}	J_{tot}
CH_3CHO	^2J(H,H)	pecJ-1	112	-16.4	-0.6	-17.0
		pecJ-2	196	-15.9		-16.5
		ccJ-pVDZ	104	-16.5		-17.1
		ccJ-pVTZ	208	-15.8		-16.4
		pcJ-1	108	-17.0		-17.6
		pcJ-2	228	-16.0		-16.6
CF_4	^2J(F,F)	pecJ-1	135	48.0	-4.9	43.1
		pecJ-2	215	34.9		30.0
		ccJ-pVDZ	125	40.0		35.1
		ccJ-pVTZ	205	40.8		35.9
		pcJ-1	135	55.9		51.0
		pcJ-2	255	39.3		34.4
CH_2F_2	^2J(F,F)	pecJ-1	103	354.8	5.9	360.7
		pecJ-2	169	332.3		338.2
		ccJ-pVDZ	95	355.7		361.6
		ccJ-pVTZ	171	344.9		350.8
		pcJ-1	101	364.2		370.1
		pcJ-2	201	334.2		340.1
	^2J(H,H)	pecJ-1	103	0.0	0.7	0.7
		pecJ-2	169	1.4		2.1
		ccJ-pVDZ	95	0.7		1.4
		ccJ-pVTZ	171	1.7		2.4
		pcJ-1	101	0.4		1.1
		pcJ-2	201	1.5		2.2
CH_3F	^1J(C,H)	pecJ-1	87	139.3	3.9	143.2
		pecJ-2	146	140.2		144.1
		ccJ-pVDZ	80	140.5		144.4
		ccJ-pVTZ	154	140.6		144.5
		pcJ-1	84	141.4		145.3
		pcJ-2	174	140.7		144.6
	^2J(F,H)	pecJ-1	87	46.4	-1.5	44.9
		pecJ-2	146	48.0		46.5
		ccJ-pVDZ	80	48.7		47.2
		ccJ-pVTZ	154	48.7		47.2
		pcJ-1	84	49.2		47.7
		pcJ-2	174	47.8		46.3
	^2J(H,H)	pecJ-1	87	-10.9	-0.2	-11.1
		pecJ-2	146	-10.1		-10.3
		ccJ-pVDZ	80	-10.6		-10.8
		ccJ-pVTZ	154	-9.9		-10.1
		pcJ-1	84	-10.9		-11.1
		pcJ-2	174	-10.2		-10.4

NH_3	^2J(H,H)	pecJ-1	60	-12.3	0.7	-11.6
		pecJ-2	103	-10.9		-10.2
		ccJ-pVDZ	55	-12.2		-11.5
		ccJ-pVTZ	113	-10.6		-9.9
		pcJ-1	57	-12.3		-11.6
		pcJ-2	123	-10.7		-10.0
CH_3CN	^2J(C,N)	pecJ-1	114	2.5	0.2	2.7
		pecJ-2	189	2.7		2.9
		ccJ-pVDZ	105	2.6		2.8
		ccJ-pVTZ	195	2.7		2.9
		pcJ-1	111	2.6		2.8
		pcJ-2	225	2.7		2.9
	^2J(H,H)	pecJ-1	114	-16.8	-0.7	-17.5
		pecJ-2	189	-16.3		-17.0
		ccJ-pVDZ	105	-17.0		-17.7
		ccJ-pVTZ	195	-16.2		-16.9
		pcJ-1	111	-17.5		-18.2
		pcJ-2	225	-16.4		-17.1
CH_3NH_2	^1J(C,H)	pecJ-1	109	124.6	4.6	129.2
		pecJ-2	186	126.0		130.6
		ccJ-pVDZ	100	126.3		130.9
		ccJ-pVTZ	202	126.2		130.8
		pcJ-1	104	126.9		131.5
		pcJ-2	222	126.2		130.8
	^2J(H-N-H)	pecJ-1	109	-11.6	0.5	-11.1
		pecJ-2	186	-10.3		-9.8
		ccJ-pVDZ	100	-11.4		-10.9
		ccJ-pVTZ	202	-10.0		-9.5
		pcJ-1	104	-11.5		-11.0
		pcJ-2	222	-10.2		-9.7
	^2J(H-C-H)	pecJ-1	109	-13.5	-0.7	-14.2
		pecJ-2	186	-13.0		-13.7
		ccJ-pVDZ	100	-13.5		-14.2
		ccJ-pVTZ	202	-12.8		-13.5
		pcJ-1	104	-14.0		-14.7
		pcJ-2	222	-13.0		-13.7
	^2J(H-N-C)	pecJ-1	109	-3.9	-0.4	-4.3
		pecJ-2	186	-3.4		-3.8
		ccJ-pVDZ	100	-4.0		-4.4
		ccJ-pVTZ	202	-3.4		-3.8
		pcJ-1	104	-3.9		-4.3
		pcJ-2	222	-3.4		-3.8
	^2J(H-C-N)	pecJ-1	109	-0.7	0.0	-0.7
		pecJ-2	186	-0.8		-0.8
		ccJ-pVDZ	100	-0.8		-0.8
		ccJ-pVTZ	202	-0.9		-0.9
		pcJ-1	104	-0.3		-0.3

		pcJ-2	222	-0.8		-0.8
	^3J(H,H)	pecJ-1	109	6.5	0.4	6.9
		pecJ-2	186	6.6		7.0
		ccJ-pVDZ	100	6.4		6.8
		ccJ-pVTZ	202	6.6		7.0
		pcJ-1	104	6.5		6.9
		pcJ-2	222	6.6		7.0

Equilibrium geometries

H2 CCSD[T]/aug-cc-pV5Z geometry:

H 0.000000 0.000000 0.000000
H 0.000000 0.000000 0.741608

C2H2 CCSD[T]/aug-cc-pV5Z geometry:

C 0.000000 0.000000 0.000000
C 0.000000 0.000000 1.201932
H 0.000000 0.000000 -1.059175
H 0.000000 0.000000 2.261107

N2 CCSD[T]/aug-cc-pVQZ geometry:

N 0.000000 0.000000 0.000000
N 0.000000 0.000000 1.098191

F2 CCSD[T]/aug-cc-pVQZ geometry:

F 0.000000 0.000000 0.000000
F 0.000000 0.000000 1.410220

CH4 CCSD[T]/aug-cc-pV5Z geometry:

C 0.000000 0.000000 0.000000
H 0.000000 0.000000 1.084304
H 1.022292 0.000000 -0.361435
H -0.511146 -0.885331 -0.361435
H -0.511146 0.885331 -0.361435

NH3 CCSD[T]/aug-cc-pV5Z geometry:

N 0.000000 0.000000 0.000000
H 0.000000 0.000000 1.009374
H 0.966374 0.000000 -0.291472
H -0.392349 -0.883148 -0.291459

HF CCSD[T]/aug-cc-pV5Z geometry:

H 0.000000 0.000000 0.000000
F 0.000000 0.000000 0.916093

CH3NH2 CCSD[T]/aug-cc-pVQZ geometry:

C -0.050248 -0.704349 0.000000
N -0.050248 0.756384 -0.000000
H -0.587350 -1.059747 -0.876853
H 0.942667 -1.163461 0.000000
H -0.587350 -1.059747 0.876853
H 0.443119 1.107253 0.808804
H 0.443119 1.107253 -0.808804

CH3F CCSD[T]/aug-cc-pVQZ geometry:

C 0.000000 0.000000 0.000000
F 0.000000 0.000000 1.381670
H 1.028869 0.000000 -0.350417
H -0.514434 -0.891027 -0.350416
H -0.514435 0.891026 -0.350417

CH3CN CCSD[T]/aug-cc-pVQZ geometry:

C 0.000000 0.000000 0.000000
C 0.000000 0.000000 1.458513
N 0.000000 0.000000 2.614443
H 0.000000 1.021083 -0.369268
H 0.884284 -0.510542 -0.369268
H -0.884284 -0.510542 -0.369268

CH3CHO CCSD[T]/aug-cc-pVQZ geometry:

C 0.000000 0.000000 0.000000
C 0.000000 0.000000 1.493631
O 0.966776 0.000000 2.169827
H -1.003217 0.000000 1.954314
H -0.538912 -0.875276 -0.361736
H -0.538912 0.875276 -0.361736
H 1.013668 0.000000 -0.385927

CF2H2 CCSD[T]/aug-cc-pVQZ geometry:

C 0.000000 0.000000 0.000000
F 0.000000 0.000000 1.353125
F 1.283765 0.000000 -0.427661
H -0.484666 -0.909444 -0.346074
H -0.485857 0.906141 -0.352997

CF4 CCSD[T]/aug-cc-pVQZ geometry:

C	0.000000	0.000000	0.000000
F	0.000000	0.000000	1.315134
F	1.239920	0.000000	-0.438378
F	-0.619960	-1.073802	-0.438378
F	-0.619960	1.073802	-0.438378

C6H6 CCSD/PCM/aug-cc-pVQZ geometry in benzene:

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.386066
C	1.200368	0.000000	2.079099
C	2.400736	0.000000	1.386066
C	2.400736	0.000000	-0.000000
C	1.200368	0.000000	-0.693033
H	-0.933380	0.000000	1.924953
H	3.334117	0.000000	-0.538887
H	3.334117	0.000000	1.924953
H	1.200368	0.000000	-1.770808
H	1.200368	0.000000	3.156874
H	-0.933380	0.000000	-0.538887

C2H6 CCSD/PCM/aug-cc-pVQZ geometry in carbon tetrachloride:

C	0.000000	0.000000	0.761933
C	0.000000	0.000000	-0.761933
H	0.000000	1.015469	1.155985
H	-0.879422	-0.507734	1.155985
H	0.879422	-0.507734	1.155985
H	0.000000	-1.015469	-1.155985
H	-0.879422	0.507734	-1.155985
H	0.879422	0.507734	-1.155985

C2H4 CCSD/PCM/aug-cc-pVQZ geometry in carbon tetrachloride:

C	0.000000	0.000000	0.664597
C	0.000000	0.000000	-0.664597
H	0.000000	0.921801	1.229229
H	0.000000	-0.921801	1.229229
H	0.000000	-0.921801	-1.229229
H	0.000000	0.921801	-1.229229