Supporting Information

for

"Efficient and Flexible Computation of Many-Electron Wave Function Overlaps"

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Table 1: Molecular coordinates (a.u.) and CASSCF(6,5)/ANO-RCC-VDZP total energies (a.u.) of selenoacroleine for $\theta = 50$.

	charge	x	y	z	mass
Se	34.0	0.00000000	0.00000000	0.00000000	79.91652050
C	6.0	3.35609824	0.00000000	0.00000000	12.00000000
C	6.0	4.91982834	0.00000000	2.23103045	12.00000000
C	6.0	7.46871085	-0.00209760	2.11282803	12.00000000
H	1.0	4.34389628	0.00073699	-1.79701688	1.00782504
H	1.0	3.96957918	0.00289128	4.04061401	1.00782504
H	1.0	8.48096195	1.33176612	0.94350284	1.00782504
H	1.0	8.58005922	-1.34225410	3.18747791	1.00782504

Total energies:

S_0	-2543.961666228
S_1	-2543.914664883
T_1	-2543.917701373
T_2	-2543.916940954

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Table 2: Molecular coordinates (a.u.) and CASSCF(6,5)/ANO-RCC-VDZP total energies (a.u.) of selenoacroleine for $\theta = 55$.

	charge	x	y	z	mass
Se	34.0	0.00000000	0.00000000	0.00000000	79.91652050
C	6.0	3.35609824	0.00000000	0.00000000	12.00000000
C	6.0	4.91982834	0.00000000	2.23103045	12.00000000
C	6.0	7.46871085	-0.00209760	2.11282803	12.00000000
H	1.0	4.34389628	0.00073699	-1.79701688	1.00782504
H	1.0	3.96957918	0.00289128	4.04061401	1.00782504
H	1.0	8.48663113	1.42440053	1.06397292	1.00782504
H	1.0	8.57437115	-1.43519087	3.06659209	1.00782504

Total energies:

S_0	-2543.953718502
S_1	-2543.911140703
T_1	-2543.916763113
T_2	-2543.913370031

Table 3: Molecular coordinates (a.u.) and CASSCF(12,9)/LANL2DZ+6-31G* total energies (a.u.) of $Ir(C_3H_4N)_3$.

	charge	x	y	z	mass
Ir	77.0	0.00000000	0.00000000	-0.01329000	192.21700000
N	7.0	1.80010200	-2.88697100	-2.13249500	14.00670000
N	7.0	-3.40024100	-0.11544800	-2.13249500	14.00670000
C	6.0	-0.90979600	3.01827600	2.02816800	12.01070000
C	6.0	3.06880100	-0.72123200	2.02816800	12.01070000
C	6.0	3.89138200	-3.69239700	-1.14545400	12.01070000
C	6.0	4.66122000	-2.55908600	1.16433200	12.01070000
N	7.0	1.60013900	3.00241900	-2.13249500	14.00670000
C	6.0	-2.15900500	-2.29704400	2.02816800	12.01070000
C	6.0	1.25201800	5.21623400	-1.14545400	12.01070000
C	6.0	-0.11437700	5.31627800	1.16433200	12.01070000
C	6.0	-5.14340000	-1.52383700	-1.14545400	12.01070000
C	6.0	-4.54684300	-2.75719200	1.16433200	12.01070000
H	1.0	3.54963500	0.20333600	3.80678600	1.00794000
H	1.0	6.37476200	-3.16092400	2.11423500	1.00794000
H	1.0	4.98544300	-5.17760000	-2.06307100	1.00794000
H	1.0	1.99121100	6.90632000	-2.06307100	1.00794000
H	1.0	-0.44994000	7.10116800	2.11423500	1.00794000
H	1.0	-1.95091200	2.97240600	3.80678600	1.00794000
H	1.0	-5.92482200	-3.94024400	2.11423500	1.00794000
H	1.0	-1.59872300	-3.17574200	3.80678600	1.00794000
H	1.0	-6.97665500	-1.72872100	-2.06307100	1.00794000
H	1.0	1.26111400	-3.71441700	-3.76807100	1.00794000
H	1.0	2.58622300	2.94936500	-3.76807100	1.00794000
H	1.0	-3.84733700	0.76505200	-3.76807100	1.00794000

Total energies:

S_0	-614.932489444
S_1	-614.780433920
S_2	-614.780433856
S_3	-614.779275581
S_4	-614.770666413
S_5	-614.770666349
S_6	-614.767439924
S_7	-614.762725810
S_8	-614.762725728
S_9	-614.705153779