property	inst	ylb	yub	#V	#C	time	n(G)	a_MILP	a_pyscf_6-31G(2df,p)	a_PSI4_6-311G(2df,p)
homo	b1	-5.00	-4.50	10517	55112	>1h				
		-5.50	-5.00	10517	55112	>1h				
		-6.00	-5.50	10517	55112	>1h				
		-6.50	-6.00	10517	55112	>1h				
		-7.00	-6.50	10517	55112	2235.537	15	-6.92995	-7.06891	-7.28995
		-7.50	-7.00	10517	55112	43.981	16	-7.25413	-7.24618	-7.50739
		-8.00	-7.50	10517	55112	40.644	19	-7.63504	-7.39256	-7.71839
		-8.50	-8.00	10517	55112	>1h				
		-9.00	-8.50	10517	55112	>1h				
		-9.50	-9.00	10517	55112	>1h				
	b2	-5.00	-4.50	10163	57570	>1h				
		-5.50	-5.00	10163	57570	>1h				
		-6.00	-5.50	10163	57570	>1h				
		-6.50	-6.00	10163	57570	>1h				
		-7.00	-6.50	10163	57570	4.134	10	-6.51518	-6.25516	-7.31864
		-7.50	-7.00	10163	57570	>1h				
		-8.00	-7.50	10163	57570	>1h				
		-8.50	-8.00	10163	57570	>1h				
		-9.00	-8.50	10163	57570	>1h				
		-9.50	-9.00	10163	57570	>1h				
	b3	-5.00	-4.50	10159	57958	>1h				
		-5.50	-5.00	10159	57958	>1h				
		-6.00	-5.50	10159	57958	>1h				
		-6.50	-6.00	10159	57958	3.968	10	-6.42172	-6.90626	maximum dynamic_level reached
		-7.00	-6.50	10159	57958	4.087	11	-6.58198	-7.13514	unable to compute torsion value
		-7.50	-7.00	10159	57958	>1h				
		-8.00	-7.50	10159	57958	>1h				
		-8.50	-8.00	10159	57958	>1h				
		-9.00	-8.50	10159	57958	>1h				
		-9.50	-9.00	10159	57958	>1h				
	b4	-5.00	-4.50	10151	58342	>1h				
		-5.50	-5.00	10151	58342	>1h				
		-6.00	-5.50	10151	58342	>1h				
		-6.50	-6.00	10151	58342	4.123	10	-6.27818	-5.87852	-6.38071
		-7.00	-6.50	10151	58342	>1h				
		-7.50	-7.00	10151	58342	>1h				
		-8.00	-7.50	10151	58342	>1h				
		-8.50	-8.00	10151	58342	4.112	14	-8.49821	-7.09838	maximum dynamic_level reached
		-9.00	-8.50	10151	58342	>1h				
		-9.50	-9.00	10151	58342	4.193	14	-9.29608	-8.59167	maximum dynamic_level reached
	e	-5.00	-4.50	7377	34508	>1h				
		-5.50	-5.00	7377	34508	>1h				
		-6.00	-5.50	7377	34508	>1h				
		-6.50	-6.00	7377	34508	57.667	9	-6.46383	-5.57832	-6.08835
		-7.00	-6.50	7377	34508	36.664	9	-6.61189		
		-7.50	-7.00	7377	34508	19.008	9	-7.01391	-5.84124	-6.36345
		-8.00	-7.50	7377	34508	>1h				
		-8.50	-8.00	7377	34508	>1h				
		-9.00	-8.50	7377	34508	2.207	9	-8.50310	-7.99018	maximum dynamic_level reached
		-9.50	-9.00	7377	34508	>1h				

property	inst	ylb	yub	#V	#C	time	n(G)	a_MILP	a_pyscf_6-31G(2df,p)	a_PSI4_6-311G(2df,p)
lumo	b1	-0.50	0.00	10517	55112	>1h				
		-1.00	-0.50	10517	55112	1072.264	16	-0.97852	-1.90723	maximum dynamic_level reached
		-1.50	-1.00	10517	55112	2643.544	18	-1.42366	-2.09032	unable to compute torsion value
		-2.00	-1.50	10517	55112	60.889	19	-1.76264	-2.01727	-2.15115
		-2.50	-2.00	10517	55112	1613.007	17	-2.24640	-1.51615	unable to compute torsion value
		-3.00	-2.50	10517	55112	330.653	16	-2.65857	-2.50482	unable to compute torsion value
		-3.50	-3.00	10517	55112	>1h				
		0.00	0.50	10517	55112	3164.133	17	0.44024	-0.50280	unable to compute torsion value
		0.50	1.00	10517	55112	1833.259	19	0.84710	0.89286	unable to compute torsion value
		1.00	1.50	10517	55112	>1h				
	b2	-0.50	0.00	10163	57570	>1h				
		-1.00	-0.50	10163	57570	>1h				
		-1.50	-1.00	10163	57570	>1h				
		-2.00	-1.50	10163	57570	>1h				
		-2.50	-2.00	10163	57570	>1h				
		-3.00	-2.50	10163	57570	>1h				
		-3.50	-3.00	10163	57570	>1h				
		0.00	0.50	10163	57570	>1h				
		0.50	1.00	10163	57570	>1h				
		1.00	1.50	10163	57570	>1h				
	b3	-0.50	0.00	10159	57958	>1h				
		-1.00	-0.50	10159	57958	>1h				
		-1.50	-1.00	10159	57958	>1h				
		-2.00	-1.50	10159	57958	>1h				
		-2.50	-2.00	10159	57958	>1h				
		-3.00	-2.50	10159	57958	>1h				
		-3.50	-3.00	10159	57958	4.013	11	-3.35504	-4.74164	unable to compute torsion value
		0.00	0.50	10159	57958	>1h				
		0.50	1.00	10159	57958	>1h				
		1.00	1.50	10159	57958	>1h				
	b4	-0.50	0.00	10151	58342	>1h				
		-1.00	-0.50	10151	58342	>1h				
		-1.50	-1.00	10151	58342	4.194	14	-1.09109	-3.00774	-1.98944
		-2.00	-1.50	10151	58342	>1h				
		-2.50	-2.00	10151	58342	>1h				
		-3.00	-2.50	10151	58342	4.297	10	-2.51701		unable to compute torsion value
		-3.50	-3.00	10151	58342	>1h				
		0.00	0.50	10151	58342	3243.109	14	0.05767	-3.58014	
		0.50	1.00	10151	58342	4.265	14	0.84079	-2.67388	-4.22520
		1.00	1.50	10151	58342	>1h				
	e	-0.50	0.00	7377	34508	>1h				
		-1.00	-0.50	7377	34508	>1h				
		-1.50	-1.00	7377	34508	209.798	9	-1.25755	-4.70795	-4.37181
		-2.00	-1.50	7377	34508	27.958	9	-1.96522		
		-2.50	-2.00	7377	34508	>1h				
		-3.00	-2.50	7377	34508	>1h				
		-3.50	-3.00	7377	34508	>1h				
		0.00	0.50	7377	34508	207.869	8	0.05622	-2.90942	-1.16513
		0.50	1.00	7377	34508	163.198	8	0.66924	0.48083	unable to compute torsion value
		1.00	1.50	7377	34508	881.593	9	1.03216	1.14088	0.73261

property	inst	ylb	yub	#V	#C	time	n(G)	a_MILP	a_pyscf_6-31G(2df,p)	a_PSI4_6-311G(2df,p)
gap	b1	4.00	4.50	10517	55112	1182.118	19	4.38198	3.36369	unable to compute torsion value
		4.50	5.00	10517	55112	2040.866	17	4.67877	4.64756	unable to compute torsion value
		5.00	5.50	10517	55112	476.513	17	5.43488	2.62759	4.24181
		5.50	6.00	10517	55112	>1h				
		6.00	6.50	10517	55112	62.145	20	6.27711	6.07699	6.28504
		6.50	7.00	10517	55112	>1h				
		7.00	7.50	10517	55112	>1h				
		7.50	8.00	10517	55112	>1h				
		8.50	9.00	10517	55112	>1h				
		9.00	9.50	10517	55112	>1h				
	b2	4.00	4.50	10163	57570	>1h				
		4.50	5.00	10163	57570	>1h				
		5.00	5.50	10163	57570	>1h				
		5.50	6.00	10163	57570	>1h				
		6.00	6.50	10163	57570	4.007	11	6.08124	2.09943	2.40124
		6.50	7.00	10163	57570	>1h				
		7.00	7.50	10163	57570	>1h				
		7.50	8.00	10163	57570	>1h				
		8.50	9.00	10163	57570	>1h				
		9.00	9.50	10163	57570	>1h				
	b3	4.00	4.50	10159	57958	>1h				
		4.50	5.00	10159	57958	>1h				
		5.00	5.50	10159	57958	>1h				
		5.50	6.00	10159	57958	>1h				
		6.00	6.50	10159	57958	>1h				
		6.50	7.00	10159	57958	>1h				
		7.00	7.50	10159	57958	>1h				
		7.50	8.00	10159	57958	>1h				
		8.50	9.00	10159	57958	>1h				
		9.00	9.50	10159	57958	>1h				
	b4	4.00	4.50	10151	58342	>1h				
		4.50	5.00	10151	58342	>1h				
		5.00	5.50	10151	58342	>1h				
		5.50	6.00	10151	58342	>1h				
		6.00	6.50	10151	58342	4.161	11	6.08124	1.47346	unable to compute torsion value
		6.50	7.00	10151	58342	>1h				
		7.00	7.50	10151	58342	>1h				
		7.50	8.00	10151	58342	>1h				
		8.50	9.00	10151	58342	>1h				
		9.00	9.50	10151	58342	>1h				
	e	4.00	4.50	7377	34508	>1h				
		4.50	5.00	7377	34508	1453.393	8	4.69120	3.19935	2.79613
		5.00	5.50	7377	34508	173.707	8	5.02681	2.82827	unable to compute torsion value
		5.50	6.00	7377	34508	23.145	9	5.59739	2.28670	unable to compute torsion value
		6.00	6.50	7377	34508	257.274	9	6.08344	3.64805	4.13713
		6.50	7.00	7377	34508	467.762	9	6.85934	2.26632	3.72492
		7.00	7.50	7377	34508	753.747	9	7.13251	6.45730	6.48175
		7.50	8.00	7377	34508	>1h				
		8.50	9.00	7377	34508	1215.420	9	8.60776	4.65990	5.46136
		9.00	9.50	7377	34508	>1h				

property	inst	ylb	yub	#V	#C	time	n(G)	a_MILP	a_pyscf_6-31G(2df,p)	a_PSI4_6-311G(2df,p)
homo	b1	-5.00	-4.50	18325	108328	>1h				
		-5.50	-5.00	18325	108328	>1h				
		-6.00	-5.50	18325	108328	>1h				
		-6.50	-6.00	18325	108328	>1h				
		-7.00	-6.50	18325	108328	>1h				
		-7.50	-7.00	18325	108328	>1h				
		-8.00	-7.50	18325	108328	>1h				
		-8.50	-8.00	18325	108328	>1h				
		-9.00	-8.50	18325	108328	>1h				
		-9.50	-9.00	18325	108328	>1h				
	b2	-5.00	-4.50	17731	113090	>1h				
		-5.50	-5.00	17731	113090	>1h				
		-6.00	-5.50	17731	113090	>1h				
		-6.50	-6.00	17731	113090	>1h				
		-7.00	-6.50	17731	113090	>1h				
		-7.50	-7.00	17731	113090	>1h				
		-8.00	-7.50	17731	113090	>1h				
		-8.50	-8.00	17731	113090	>1h				
		-9.00	-8.50	17731	113090	>1h				
		-9.50	-9.00	17731	113090	>1h				
	b3	-5.00	-4.50	17823	113862	>1h				
		-5.50	-5.00	17823	113862	>1h				
		-6.00	-5.50	17823	113862	>1h				
		-6.50	-6.00	17823	113862	>1h				
		-7.00	-6.50	17823	113862	>1h				
		-7.50	-7.00	17823	113862	>1h				
		-8.00	-7.50	17823	113862	>1h				
		-8.50	-8.00	17823	113862	>1h				
		-9.00	-8.50	17823	113862	>1h				
		-9.50	-9.00	17823	113862	>1h				
	b4	-5.00	-4.50	17911	114630	>1h				
		-5.50	-5.00	17911	114630	>1h				
		-6.00	-5.50	17911	114630	>1h				
		-6.50	-6.00	17911	114630	>1h				
		-7.00	-6.50	17911	114630	>1h				
		-7.50	-7.00	17911	114630	>1h				
		-8.00	-7.50	17911	114630	>1h				
		-8.50	-8.00	17911	114630	>1h				
		-9.00	-8.50	17911	114630	>1h				
		-9.50	-9.00	17911	114630	>1h				
	e	-5.00	-4.50	12785	67516	>1h				
		-5.50	-5.00	12785	67516	>1h				
		-6.00	-5.50	12785	67516	3262.404	9	-5.51096	-6.01995	unable to compute torsion value
		-6.50	-6.00	12785	67516	958.843	9	-6.49501	-5.57832	-6.08822
		-7.00	-6.50	12785	67516	1055.130	9	-6.99548		
		-7.50	-7.00	12785	67516	>1h				
		-8.00	-7.50	12785	67516	>1h				
		-8.50	-8.00	12785	67516	6.323	9	-8.21541	-7.99018	maximum dynamic_level reached
		-9.00	-8.50	12785	67516	>1h				
		-9.50	-9.00	12785	67516	>1h				

property	inst	ylb	yub	#V	#C	time	n(G)	a_MILP	a_pyscf_6-31G(2df,p)	a_PSI4_6-311G(2df,p)
lumo	b1	-0.50	0.00	18325	108328	>1h				
		-1.00	-0.50	18325	108328	>1h				
		-1.50	-1.00	18325	108328	>1h				
		-2.00	-1.50	18325	108328	>1h				
		-2.50	-2.00	18325	108328	>1h				
		-3.00	-2.50	18325	108328	>1h				
		-3.50	-3.00	18325	108328	>1h				
		0.00	0.50	18325	108328	>1h				
		0.50	1.00	18325	108328	>1h				
		1.00	1.50	18325	108328	>1h				
	b2	-0.50	0.00	17731	113090	>1h				
		-1.00	-0.50	17731	113090	>1h				
		-1.50	-1.00	17731	113090	>1h				
		-2.00	-1.50	17731	113090	>1h				
		-2.50	-2.00	17731	113090	>1h				
		-3.00	-2.50	17731	113090	>1h				
		-3.50	-3.00	17731	113090	>1h				
		0.00	0.50	17731	113090	>1h				
		0.50	1.00	17731	113090	>1h				
		1.00	1.50	17731	113090	>1h				
	b3	-0.50	0.00	17823	113862	>1h				
		-1.00	-0.50	17823	113862	>1h				
		-1.50	-1.00	17823	113862	>1h				
		-2.00	-1.50	17823	113862	>1h				
		-2.50	-2.00	17823	113862	>1h				
		-3.00	-2.50	17823	113862	>1h				
		-3.50	-3.00	17823	113862	>1h				
		0.00	0.50	17823	113862	>1h				
		0.50	1.00	17823	113862	>1h				
		1.00	1.50	17823	113862	>1h				
	b4	-0.50	0.00	17911	114630	>1h				
		-1.00	-0.50	17911	114630	>1h				
		-1.50	-1.00	17911	114630	>1h				
		-2.00	-1.50	17911	114630	>1h				
		-2.50	-2.00	17911	114630	>1h				
		-3.00	-2.50	17911	114630	>1h				
		-3.50	-3.00	17911	114630	>1h				
		0.00	0.50	17911	114630	>1h				
		0.50	1.00	17911	114630	>1h				
		1.00	1.50	17911	114630	>1h				
	e	-0.50	0.00	12785	67516	6.417	9	-0.43834	-0.76486	-2.65267
		-1.00	-0.50	12785	67516	2682.617	9	-0.68091	-2.24580	-2.20569
		-1.50	-1.00	12785	67516	>1h				
		-2.00	-1.50	12785	67516	>1h				
		-2.50	-2.00	12785	67516	373.309	9	-2.28381	-3.49353	-2.73663
		-3.00	-2.50	12785	67516	293.280	9	-2.78664	-3.41432	-3.08009
		-3.50	-3.00	12785	67516	293.516	9	-3.25859		
		0.00	0.50	12785	67516	>1h				
		0.50	1.00	12785	67516	>1h				
		1.00	1.50	12785	67516	6.355	9	1.49046	1.53046	maximum dynamic_level reached

property	inst	ylb	yub	#V	#C	time	n(G)	a_MILP	a_pyscf_6-31G(2df,p)	a_PSI4_6-311G(2df,p)
gap	b1	4.00	4.50	18325	108328	>1h				
		4.50	5.00	18325	108328	618.418	17	4.98681	4.86001	5.13423
		5.00	5.50	18325	108328	>1h				
		5.50	6.00	18325	108328	>1h				
		6.00	6.50	18325	108328	>1h				
		6.50	7.00	18325	108328	>1h				
		7.00	7.50	18325	108328	>1h				
		7.50	8.00	18325	108328	>1h				
		8.50	9.00	18325	108328	>1h				
		9.00	9.50	18325	108328	>1h				
	b2	4.00	4.50	17731	113090	>1h				
		4.50	5.00	17731	113090	>1h				
		5.00	5.50	17731	113090	>1h				
		5.50	6.00	17731	113090	>1h				
		6.00	6.50	17731	113090	>1h				
		6.50	7.00	17731	113090	>1h				
		7.00	7.50	17731	113090	>1h				
		7.50	8.00	17731	113090	>1h				
		8.50	9.00	17731	113090	>1h				
		9.00	9.50	17731	113090	>1h				
	b3	4.00	4.50	17823	113862	>1h				
		4.50	5.00	17823	113862	>1h				
		5.00	5.50	17823	113862	11.400	10	5.23926	2.99164	3.04533
		5.50	6.00	17823	113862	>1h				
		6.00	6.50	17823	113862	>1h				
		6.50	7.00	17823	113862	>1h				
		7.00	7.50	17823	113862	>1h				
		7.50	8.00	17823	113862	>1h				
		8.50	9.00	17823	113862	>1h				
		9.00	9.50	17823	113862	>1h				
	b4	4.00	4.50	17911	114630	>1h				
		4.50	5.00	17911	114630	>1h				
		5.00	5.50	17911	114630	>1h				
		5.50	6.00	17911	114630	>1h				
		6.00	6.50	17911	114630	>1h				
		6.50	7.00	17911	114630	>1h				
		7.00	7.50	17911	114630	>1h				
		7.50	8.00	17911	114630	11.961	14	7.73886	5.26669	maximum dynamic_level reached
		8.50	9.00	17911	114630	>1h				
		9.00	9.50	17911	114630	11.722	14	9.08023	5.46993	6.71495
	e	4.00	4.50	12785	67516	338.436	9	4.16292	2.13027	unable to compute torsion value
		4.50	5.00	12785	67516	2669.096	9	4.98732	3.92076	4.62589
		5.00	5.50	12785	67516	>1h				
		5.50	6.00	12785	67516	2293.533	9	5.81378	2.23462	unable to compute torsion value
		6.00	6.50	12785	67516	3375.859	8	6.24128	2.26631	unable to compute torsion value
		6.50	7.00	12785	67516	2333.743	9	6.91824	1.27482	4.33042
		7.00	7.50	12785	67516	624.329	9	7.12222	4.18467	4.87739
		7.50	8.00	12785	67516	>1h				
		8.50	9.00	12785	67516	>1h				
		9.00	9.50	12785	67516	>1h				