Willem Klopper

List of Publications by Citations

306 papers	20,483 citations	66 h-index	135 g-index
334 ext. papers	21,912 ext. citations	4.3 avg, IF	6.84 L-index

#	Paper	IF	Citations
306	Basis-set convergence of correlated calculations on water. *Journal of Chemical Physics*, **1997**, 106, 9639-9646	3.9	1932
305	Basis-set convergence in correlated calculations on Ne, N2, and H2O. *Chemical Physics Letters*, **1998**, 286, 243-252	2.5	1786
304	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
303	Turbomole. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 91-100	7.9	710
302	Basis-set convergence of the energy in molecular HartreeFock calculations. *Chemical Physics Letters*, **1999**, 302, 437-446	2.5	535
301	Wave functions with terms linear in the interelectronic coordinates to take care of the correlation cusp. I. General theory. *Journal of Chemical Physics*, **1991**, 94, 1985-2001	3.9	496
300	Explicitly correlated electrons in molecules. *Chemical Reviews*, **2012**, 112, 4-74	68.1	419
299	Optimized accurate auxiliary basis sets for RI-MP2 and RI-CC2 calculations for the atoms Rb to Rn. *Theoretical Chemistry Accounts*, **2007**, 117, 587-597	1.9	396
298	R12 methods in explicitly correlated molecular electronic structure theory. *International Reviews in Physical Chemistry*, **2006**, 25, 427-468	7	360
297	Basis set convergence of the interaction energy of hydrogen-bonded complexes. *Journal of Chemical Physics*, **1999**, 111, 9157-9167	3.9	333
296	Explicitly correlated second-order MllerPlesset methods with auxiliary basis sets. *Journal of Chemical Physics*, **2002**, 116, 6397-6410	3.9	292
295	Synthesis, structure, and characterization of dinuclear copper(I) halide complexes with P^N ligands featuring exciting photoluminescence properties. *Inorganic Chemistry*, **2013**, 52, 2292-305	5.1	282
294	Mller-plesset calculations taking care of the correlation CUSP. *Chemical Physics Letters*, **1987**, 134, 17-22	2.5	259
293	Computational determination of equilibrium geometry and dissociation energy of the water dimer. *Physical Chemistry Chemical Physics*, **2000**, 2, 2227-2234	3.6	235
292	Quintuple-zeta quality coupled-cluster correlation energies with triple-zeta basis sets. *Physical Chemistry Chemical Physics*, **2007**, 9, 1921-30	3.6	223
291	New correlation factors for explicitly correlated electronic wave functions. *Journal of Chemical Physics*, **2005**, 123, 074101	3.9	220
290	CC-R12, a correlation cusp corrected coupled-cluster method with a pilot application to the Be2 potential curve. *Chemical Physics Letters*, **1992**, 199, 497-504	2.5	220

289	Accuracy of atomization energies and reaction enthalpies in standard and extrapolated electronic wave function/basis set calculations. *Journal of Chemical Physics*, **2000**, 112, 9229-9242	3.9	208
288	Basis-set extrapolation techniques for the accurate calculation of molecular equilibrium geometries using coupled-cluster theory. *Journal of Chemical Physics*, **2006**, 125, 44108	3.9	203
287	Highly accurate coupled-cluster singlet and triplet pair energies from explicitly correlated calculations in comparison with extrapolation techniques. *Molecular Physics*, **2001**, 99, 481-507	1.7	203
286	Highly accurate calculations of molecular electronic structure. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1999**, 32, R103-R130	1.3	200
285	A priori calculation of molecular properties to chemical accuracy. *Journal of Physical Organic Chemistry*, **2004**, 17, 913-933	2.1	194
284	Quantitative quantum chemistry. *Molecular Physics*, **2008**, 106, 2107-2143	1.7	179
283	On the Interaction of Dihydrogen with Aromatic Systems *Journal of Physical Chemistry A*, **2004**, 108, 3019-3023	2.8	169
282	Ab initio study of the interactions between CO(2) and N-containing organic heterocycles. *ChemPhysChem*, **2009**, 10, 374-83	3.2	164
281	Coupled-cluster theory with simplified linear-r(12) corrections: the CCSD(R12) model. *Journal of Chemical Physics*, **2005**, 122, 84107	3.9	158
280	HF dimer: Empirically refined analytical potential energy and dipole hypersurfaces from ab initio calculations. *Journal of Chemical Physics*, **1998**, 108, 10096-10115	3.9	146
279	Wave functions with terms linear in the interelectronic coordinates to take care of the correlation cusp. II. Second-order Mo/llerPlesset (MP2-R12) calculations on closed-shell atoms. *Journal of Chemical Physics*, **1991**, 94, 2002-2019	3.9	144
278	Limiting values for Mo/llerPlesset second-order correlation energies of polyatomic systems: A benchmark study on Ne, HF, H2O, N2, and He...He. *Journal of Chemical Physics*, **1995**, 102, 6168-6179	3.9	141
277	Magnetically induced current densities in aromatic, antiaromatic, homoaromatic, and nonaromatic hydrocarbons. *Journal of Physical Chemistry A*, **2009**, 113, 8668-76	2.8	138
276	Orbital-invariant formulation of the MP2-R12 method. *Chemical Physics Letters*, **1991**, 186, 583-585	2.5	136
275	Self-consistent treatment of spin-orbit interactions with efficient Hartree-Fock and density functional methods. *Physical Chemistry Chemical Physics*, **2008**, 10, 1748-56	3.6	125
274	Wave functions with terms linear in the interelectronic coordinates to take care of the correlation cusp. III. Second-order Mo/llerPlesset (MP2-R12) calculations on molecules of first row atoms. *Journal of Chemical Physics*, **1991**, 94, 2020-2030	3.9	124
273	An ab initio derived torsional potential energy surface for (H2O)3. II. Benchmark studies and interaction energies. *Journal of Chemical Physics*, **1995**, 103, 1085-1098	3.9	121
272	MP2-R12 calculations on the relative stability of carbocations. *The Journal of Physical Chemistry*, **1990**, 94, 5625-5630		116

271	Anatomy of relativistic energy corrections in light molecular systems. *Molecular Physics*, **2001**, 99, 1769-1794	1.7	115
270	A diagonal orbital-invariant explicitly-correlated coupled-cluster method. *Chemical Physics Letters*, **2008**, 452, 326-332	2.5	113
269	Potential energy surface of the H+3 ground state in the neighborhood of the minimum with microhartree accuracy and vibrational frequencies derived from it. *Journal of Chemical Physics*, **1994**, 101, 2231-2243	3.9	111
268	Basis-set convergence of the molecular electric dipole moment. *Journal of Chemical Physics*, **1999**, 111, 4424-4430	3.9	102
267	Synthesis and properties of para-substituted NCN-pincer palladium and platinum complexes. *Chemistry - A European Journal*, **2004**, 10, 1331-44	4.8	101
266	Gaussian basis sets and the nuclear cusp problem. *Computational and Theoretical Chemistry*, **1986**, 135, 339-356		99
265	An explicitly correlated coupled cluster calculation of the helium–helium interatomic potential. *Journal of Chemical Physics*, **1995**, 103, 6127-6132	3.9	98
264	CH5+: The story goes on. An explicitly correlated coupled-cluster study. *Journal of Chemical Physics*, **1997**, 106, 1863-1869	3.9	95
263	Strong N-H...pi hydrogen bonding in amide-benzene interactions. *Journal of Physical Chemistry B*, **2009**, 113, 2937-43	3.4	94
262	The MP2-F12 method in the Turbomole program package. *Journal of Computational Chemistry*, **2011**, 32, 2492-513	3.5	92
261	Synthesis of a pentasilapropellane. Exploring the nature of a stretched silicon-silicon bond in a nonclassical molecule. *Journal of the American Chemical Society*, **2010**, 132, 10264-5	16.4	88
260	Low-lying stationary points and torsional interconversions of cyclic (H2O)4: An ab initio study. *Journal of Chemical Physics*, **1995**, 103, 6114-6126	3.9	88
259	Accurate benchmark calculation of the reaction barrier height for hydrogen abstraction by the hydroperoxyl radical from methane. Implications for C(n)H(2n+2) where n = 2 --> 4. *Journal of Physical Chemistry A*, **2008**, 112, 7047-54	2.8	87
258	Basis set limit coupled cluster study of h-bonded systems and assessment of more approximate methods. *Journal of Physical Chemistry A*, **2007**, 111, 11122-33	2.8	85
257	The MP2 limit correction applied to coupled cluster calculations of the electronic dissociation energies of the hydrogen fluoride and water dimers. *Molecular Physics*, **1999**, 96, 559-570	1.7	85
256	Atomization energies from coupled-cluster calculations augmented with explicitly-correlated perturbation theory. *Chemical Physics*, **2009**, 356, 14-24	2.3	84
255	Basis set limit CCSD(T) harmonic vibrational frequencies. *Journal of Physical Chemistry A*, **2007**, 111, 11249-11288	2.8	82
254	Ab initio computations close to the one-particle basis set limit on the weakly bound van der Waals complexes benzene–neon and benzene–argon. *Journal of Chemical Physics*, **1994**, 101, 9747-9754	3.9	82

253	Multiple basis sets in calculations of triples corrections in coupled-cluster theory. *Theoretical Chemistry Accounts*, **1997**, 97, 164-176	1.9	79
252	Scope and limitations of the SCS-MP2 method for stacking and hydrogen bonding interactions. *Physical Chemistry Chemical Physics*, **2008**, 10, 2758-66	3.6	78
251	A new ab initio based six-dimensional semi-empirical pair interaction potential for HF. *Chemical Physics Letters*, **1996**, 261, 35-44	2.5	78
250	Simple recipe for implementing computation of first-order relativistic corrections to electron correlation energies in framework of direct perturbation theory. *Journal of Computational Chemistry*, **1997**, 18, 20-27	3.5	77
249	Towards the one-particle basis set limit of second-order correlation energies: MP2-R12 calculations on small Ben and Mgn clusters (n=1). *Journal of Chemical Physics*, **1993**, 99, 5167-5177	3.9	76
248	CID and CEPA calculations with linear r12 terms. *Chemical Physics Letters*, **1991**, 178, 455-461	2.5	72
247	Snapshots of the Al-Al sigma-bond formation starting from {AlR2} units: experimental and computational observations. *Angewandte Chemie - International Edition*, **2009**, 48, 8141-5	16.4	71
246	Electron correlation: the many-body problem at the heart of chemistry. *Journal of Computational Chemistry*, **2007**, 28, 1307-20	3.5	69
245	Accuracy of spectroscopic constants of diatomic molecules from ab initio calculations. *Journal of Chemical Physics*, **2003**, 118, 2539	3.9	69
244	A comparison of linear and nonlinear correlation factors for basis set limit M ller-Plesset second order binding energies and structures of He2, Be2, and Ne2. *Journal of Chemical Physics*, **2006**, 125, 094302	3.9	68
243	Expanding the coordination cage: a ruthenium(II)-polypyridine complex exhibiting high quantum yields under ambient conditions. *Inorganic Chemistry*, **2009**, 48, 5677-84	5.1	67
242	Switchable open-cage fullerene for water encapsulation. *Angewandte Chemie - International Edition*, **2010**, 49, 9935-8	16.4	67
241	Inclusion of the (T) triples correction into the linear-r12 corrected coupled-cluster model CCSD(R12). *International Journal of Quantum Chemistry*, **2006**, 106, 2306-2317	2.1	66
240	The accuracy of atomization energies from explicitly correlated coupled-cluster calculations. *Journal of Chemical Physics*, **2001**, 115, 2022-2032	3.9	66
239	Towards the accurate computation of properties of transition metal compounds: the binding energy of ferrocene. *Chemical Physics Letters*, **1996**, 262, 546-552	2.5	66
238	Experimental and Theoretical Study of Novel Luminescent Di-, Tri-, and Tetranuclear Copper Triazole Complexes. *Organometallics*, **2011**, 30, 3275-3283	3.8	65
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236	The barrier to linearity of water. *Journal of Chemical Physics*, **1999**, 110, 11971-11981	3.9	65

235	Molecular Hydrogen Interaction with IRMOF-1: A Multiscale Theoretical Study. *Journal of Physical Chemistry C*, **2007**, 111, 13635-13640	3.8	64
234	Assessment of various density functionals and basis sets for the calculation of molecular anharmonic force fields. *International Journal of Quantum Chemistry*, **2005**, 104, 830-845	2.1	64
233	Nucleobase-fluorobenzene interactions: hydrogen bonding wins over pi stacking. *Angewandte Chemie - International Edition*, **2007**, 46, 7449-52	16.4	62
232	The performance of the explicitly correlated coupled cluster method. I. The four-electron systems Be, Li and LiH. *Journal of Chemical Physics*, **1995**, 103, 309-320	3.9	61
231	An ab initio derived torsional potential energy surface for (H2O)3. I. Analytical representation and stationary points. *Journal of Chemical Physics*, **1995**, 103, 1077-1084	3.9	60
230	Robust fitting techniques in the chain of spheres approximation to the Fock exchange: The role of the complementary space. *Journal of Chemical Physics*, **2013**, 139, 094111	3.9	59
229	Coupled-cluster and explicitly correlated perturbation-theory calculations of the uracil anion. *Journal of Chemical Physics*, **2007**, 126, 085101	3.9	59
228	Coupled-cluster reference values for the GW27 and GW100 test sets for the assessment of GW methods. *Molecular Physics*, **2015**, 113, 1952-1960	1.7	57
227	para-Functionalized NCN-Pincer Palladium(II) Complexes: Synthesis, Catalysis and DFT Calculations. *European Journal of Inorganic Chemistry*, **2003**, 2003, 830-838	2.3	57
226	A hybrid scheme for the resolution-of-the-identity approximation in second-order Møller-Plesset linear-r(12) perturbation theory. *Journal of Chemical Physics*, **2004**, 120, 10890-5	3.9	56
225	ortho-Perfluoroalkylation and ethoxycarbonyldifluoromethylation of aromatic triazenes. *Journal of Organic Chemistry*, **2013**, 78, 7938-48	4.2	54
224	Accurate computational thermochemistry from explicitly correlated coupled-cluster theory. *Theoretical Chemistry Accounts*, **2010**, 126, 289-304	1.9	54
223	Basis-set extensions for two-component spin-orbit treatments of heavy elements. *Physical Chemistry Chemical Physics*, **2006**, 8, 4862-5	3.6	54
222	Computation of some new two-electron Gaussian integrals. *Theoretica Chimica Acta*, **1992**, 83, 441-453		54
221	Equilibrium inversion barrier of NH3 from extrapolated coupled-cluster pair energies. *Journal of Computational Chemistry*, **2001**, 22, 1306-1314	3.5	53
220	Anharmonic force fields and thermodynamic functions using density functional theory. *Molecular Physics*, **2005**, 103, 863-876	1.7	52
219	Anharmonic force field, vibrational energies, and barrier to inversion of SiH3 *Journal of Chemical Physics*, **2000**, 112, 4053-4063	3.9	52
218	Oriented circular dichroism analysis of chiral surface-anchored metal-organic frameworks grown by liquid-phase epitaxy and upon loading with chiral guest compounds. *Chemistry - A European Journal*, **2014**, 20, 9879-82	4.8	51

217	Cleavage of the N2 triple bond by the Ti dimer: a route to molecular materials for dinitrogen activation?. *Angewandte Chemie - International Edition*, **2006**, 45, 2799-802	16.4	50
216	Experimental and Theoretical Determination of Dissociation Energies of Dispersion-Dominated Aromatic Molecular Complexes. *Chemical Reviews*, **2016**, 116, 5614-41	68.1	50
215	Accuracy Assessment of GW Starting Points for Calculating Molecular Excitation Energies Using the Bethe-Salpeter Formalism. *Journal of Chemical Theory and Computation*, **2018**, 14, 2127-2136	6.4	49
214	Exploring the Boundary between Aromatic and Olefinic Character: Bad News for Second-Order Perturbation Theory and Density Functional Schemes. *Journal of the American Chemical Society*, **1996**, 118, 3519-3520	16.4	49
213	Two-dimensional model treatment of torsional motions in the water trimer. *Chemical Physics Letters*, **1995**, 237, 536-544	2.5	49
212	Configuration interaction calculations with terms linear in the interelectronic coordinate for the ground state of H+3. A benchmark study. *Journal of Chemical Physics*, **1993**, 99, 8830-8839	3.9	48
211	Coupled-cluster response theory with linear-r12 corrections: the CC2-R12 model for excitation energies. *Journal of Chemical Physics*, **2006**, 124, 044112	3.9	46
210	Ab initio calculation of proton barrier and binding energy of the (H2O)OH□complex. *Computational and Theoretical Chemistry*, **2002**, 586, 201-208		46
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208	Ab Initio Study of the Adsorption of Small Molecules on Metal-Organic Frameworks with Oxo-centered Trimetallic Building Units: The Role of the Undercoordinated Metal Ion. *Inorganic Chemistry*, **2015**, 54, 8251-63	5.1	43
207	High-level ab initio computations of structures and relative energies of two isomers of the CO2 trimer. *Journal of Chemical Physics*, **1999**, 111, 3846-3854	3.9	43
206	Spin flipping in ring-coupled-cluster-doubles theory. *Chemical Physics Letters*, **2011**, 510, 147-153	2.5	41
205	Accurate quantum-chemical prediction of enthalpies of formation of small molecules in the gas phase. *ChemPhysChem*, **2003**, 4, 32-48	3.2	41
204	An accurate, global, ab initio potential energy surface for the H+ 3 molecule. *Molecular Physics*, **2000**, 98, 261-273	1.7	41
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202	Second-order M□ller□Plesset perturbation theory with terms linear in the interelectronic coordinates and exact evaluation of three-electron integrals. *Theoretical Chemistry Accounts*, **2002**, 107, 173-179	1.9	40
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200	The formal combination of three singlet biradicaloid entities to a singlet hexaradicaloid metalloid Ge14[Si(SiMe3)3]5[Li(THF)2]3 cluster. *Journal of the American Chemical Society*, **2011**, 133, 2518-24	16.4	39

199	Parity-violating interaction in H2O2 calculated from density-functional theory. *Chemical Physics Letters*, **2002**, 354, 274-282	2.5	39
198	Explicitly Correlated Coupled-Cluster Theory. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 535-572	0.7	39
197	Open-shell explicitly correlated F12 methods. *Molecular Physics*, **2010**, 108, 315-325	1.7	38
196	Pentagerma[1.1.1]propellane: a combined experimental and quantum chemical study on the nature of the interactions between the bridgehead atoms. *Angewandte Chemie - International Edition*, **2009**, 48, 1411-6	16.4	38
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183	Accurate molecular geometries of the protonated water dimer. *Physical Chemistry Chemical Physics*, **2000**, 2, 2235-2238	3.6	33
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180	An improved ab initio relativistic zeroth-order regular approximation correct to order 1/c2. *Journal of Chemical Physics*, **2000**, 113, 9957-9965	3.9	32
179	Explicitly correlated coupled cluster calculations of the dissociation energies and barriers to concerted hydrogen exchange of (HF)n oligomers (n = 2,3,4,5). *Molecular Physics*, **1998**, 94, 105-119	1.7	31
178	Ionized, electron-attached, and excited states of molecular systems with spin-orbit coupling: Two-component GW and Bethe-Salpeter implementations. *Journal of Chemical Physics*, **2019**, 150, 204116	3.9	30
177	[2.2]Paracyclophanediyldiphosphane Complexes of Gold. *European Journal of Inorganic Chemistry*, **2012**, 2012, 5033-5042	2.3	30
176	Effects of counterpoise correction and basis set extrapolation on the MP2 geometries of hydrogen bonded dimers of ammonia, water, and hydrogen fluoride. *Physical Chemistry Chemical Physics*, **2011**, 13, 1230-8	3.6	30
175	Low-lying absorption and emission spectra of pyrene, 1,6-dithiapyrene, and tetrathiafulvalene: A comparison between ab initio and time-dependent density functional methods. *Journal of Chemical Physics*, **2009**, 131, 224315	3.9	30
174	Direct perturbation theory of magnetic properties and relativistic corrections for the point nuclear and Gaussian nuclear models. *Journal of Chemical Physics*, **2001**, 115, 7356-7363	3.9	30
173	The barrier to linearity of hydrogen sulphide. *Chemical Physics Letters*, **2000**, 322, 119-128	2.5	30
172	Explicitly correlated coupled cluster calculations of the dissociation energies and barriers to concerted hydrogen exchange of (HF)n oligomers (n=2,3,4,5). *Molecular Physics*, **1998**, 94, 105-119	1.7	30
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167	Ab Initio Modeling of Methanol Interaction with Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry C*, **2007**, 111, 18917-18926	3.8	29
166	Second-order electron-correlation and self-consistent spin-orbit treatment of heavy molecules at the basis-set limit. *Journal of Chemical Physics*, **2010**, 132, 094108	3.9	28
165	Extrapolation to the limit of a complete basis set for electronic structure calculations on the N2 molecule. *Theoretical Chemistry Accounts*, **1998**, 99, 265-271	1.9	28
164	Isomeric Al2R4, Mg2R2 Species and Oligomerisation Products: Investigation of Al–Al and Mg–Mg Bonding. *European Journal of Inorganic Chemistry*, **2008**, 2008, 4879-4890	2.3	28

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159	Accurate computational determination of the binding energy of the SO3 x H2O complex. *Journal of Chemical Physics*, **2006**, 125, 054312	3.9	26
158	Coinage Metal Complexes of Tris(pyrazolyl)methanide-Based Redox-Active Metalloligands. *Organometallics*, **2014**, 33, 941-951	3.8	25
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154	Nucleophilic additions to alkylidene bis(sulfoxides): stereoelectronic effects in vinyl sulfoxides. *Chemistry - A European Journal*, **2008**, 14, 4631-9	4.8	25
153	Low-lying electronic states of the Ti2 dimer: electronic absorption spectroscopy in rare gas matrices in concert with quantum chemical calculations. *Journal of Chemical Physics*, **2004**, 121, 7195-206	3.9	25
152	Extremal Electron Pairs □Application to Electron Correlation, Especially the R12 Method. *Topics in Current Chemistry*, **1999**, 21-42		25
151	Ab Initio Calculations of the Binding Energies of Small (H2O)n Clusters (n = 1□4). *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1995**, 99, 469-473		25
150	Non-covalent Interactions of CO□with Functional Groups of Metal-Organic Frameworks from a CCSD(T) Scheme Applicable to Large Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 1574-84	6.4	24
149	The geminal basis in explicitly correlated wave functions. *Chemical Physics*, **2009**, 356, 25-30	2.3	24
148	Switchable Open-Cage Fullerene for Water Encapsulation. *Angewandte Chemie*, **2010**, 122, 10131-10134	3.6	24
147	Reactivity of titanium dimer and molecular nitrogen in rare gas matrices. Vibrational and electronic spectra and structure of Ti2N2. *Physical Chemistry Chemical Physics*, **2006**, 8, 2000-11	3.6	24
146	A closed-shell coupled-cluster treatment of the Breit-Pauli first-order relativistic energy correction. *Journal of Chemical Physics*, **2004**, 121, 6591-8	3.9	24

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144	Modeling the Histidine-Phenylalanine Interaction: The NH Hydrogen Bond of Imidazole Benzene. *Journal of Physical Chemistry B*, **2015**, 119, 7778-90	3.4	22
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