Preparing a lecture on theoretical chemistry
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Combine search tools and post-processing to find information to support preparation of a lecture on theoretical chemistry.

Search objective
Find references in Reaxys that include quantum chemical calculations of alkali metal ions.
1. Perform a **Substance search**.

**Reaxys** has a unique database structure that links substance records directly with property information and corresponding references. Thus, a list of references that include quantum chemical calculations for a particular substance group is quickly found with a substance search.

To quickly build a full or part molecular formula, access the **Formula Builder** by clicking **Molecular Formula**.
2. Use **Formula Builder** to define a generic formula for alkali metal cations.

A full or part molecular formula can be quickly constructed in **Formula Builder**. Individual elements can be added by clicking on the corresponding symbol. Alternatively, click on period or group designations to include all elements in a particular row or column of the periodic table. The formula may contain number ranges as well as truncation (*).

The special groups methyl, ethyl and phenyl can also be added to a formula.

Include all elements of a particular group with a single click. **Alkali Metals** inserts “(alk)” into the formula and instructs Reaxys to include all alkali metals in the search. Adding “(1+)” to the formula instructs Reaxys to search for single-charge cations.
3. Upon clicking **Use this Formula**, a **Querylet** is added to the query form with the formula.

Click **Add/Remove Fields** to modify the query form and restrict hits to those containing quantum chemical calculations.
4. Find the **Querylet** for quantum chemical calculations and add it to the form. With >500 data fields, Reaxys includes information on a broad range of property data, from spectral and physical to ecological and bioactivity.

Type in a property type to find relevant **Querylets**. Reaxys helps with **auto-suggest**.

In this case, select the **exists** Querylet. Reaxys will retrieve literature records that include quantum chemical calculations. To specify type and method of calculation, use the Querylet **Method**.

5. The **Querylet** becomes part of the query form. Click the **exists** check box and run the search.
Reaxys retrieves 8 substance records, all single-charge cations of alkali metals and a couple isotopes.

Each substance record includes a list of property data relevant to that substance. Click on a property type to reveal excerpted data included in Reaxys, as well as references.
6. **Reaxys** includes references containing a wide range of quantum chemical calculations for Na$^{+}$.

<table>
<thead>
<tr>
<th>Calculated Properties</th>
<th>Method</th>
<th>Reference</th>
</tr>
</thead>
</table>
| Polarizability, polarizability derivatives | Ab initio calcs. (LCOA, GO SCF, DIM, SAMQ, X-alpha, Hartree-Fock) | Pearson, Erik W.; Jackson, Mark D.; Gordon, Roy G.  
  Journal of Physical Chemistry, 1984, vol. 88, # 1, p. 119 - 128  
  Title/Abstract Full Text View citing articles Show Details |
| Masses, vibrational properties          | Ab initio calcs. (LCOA, GO SCF, DIM, SAMQ, X-alpha, Hartree-Fock) | Musteler, Wolfgang; Floeh, Joachim; Meyer, Wilfried  
  Journal of Chemical Physics, 1984, vol 80, # 7 p. 3297 - 3310  
  Title/Abstract Full Text View citing articles Show Details |
| Molecular orbitals                      | Ab initio calcs. (LCOA, GO SCF, DIM, SAMQ, X-alpha, Hartree-Fock) | Fuentetoba, P.  
  Journal of Chemical Physics, 1995, vol. 103, # 15 p. 6571 - 6575  
  Title/Abstract Full Text View citing articles Show Details |
| Electronic energy levels, Total energy  | Ab initio calcs. (LCOA, GO SCF, DIM, SAMQ, X-alpha, Hartree-Fock) | Ferreira, Antonio M.; Kurtz, Henry A.; Kenna, Shashi P.  
  Title/Abstract Full Text View citing articles Show Details |
| NMR shifts, signals, intensities, transition moments | Ab initio calcs. (LCOA, GO SCF, DIM, SAMQ, X-alpha, Hartree-Fock) | Smallwood, C. Jay; Larsen, Ross E.; Glover, William J.; Schwartz, Benjamin J.  
  Journal of Chemical Physics, 2006, vol. 125, # 7 art. no. 074102  
  Title/Abstract Full Text View citing articles Show Details |
| Shielding constants                     | Electron correlation and CI calc. | Xie, Yaoming; Schreiner, Peter J.; Schaefer III, Henry F.; Li, Xiao-Wang; Robinson, Gregory H.  
  Title/Abstract Full Text View citing articles Show Details |
| UV/VIS wave lengths                     | Ab initio calcs. (LCOA, GO SCF, DIM, SAMQ, X-alpha, Hartree-Fock) | Ochterski, Joseph W.; Peterson; Montgomery Jr.  
  Title/Abstract Full Text View citing articles Show Details |
| Ionization potentials, orbital energy   | Electron correlation and CI calc. | Winter, Bernd; Weber, Ramona; Hertel, Ingolf V.; Feubel, Manfred; Jungwirth, Pavel; Brown, Eric C.; Bradforth, Stephen E.  
  Title/Abstract Full Text View citing articles Show Details |

References are organized by calculated property type and method. Thus, it is possible to go directly to references containing information of interest, instead of sifting through reference lists containing a mixture of property types.

View the title and abstract of citations, the full text or citing articles.
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