

View Job 99922: CH3ON, Molecular Energy - Gaussian


Status <<

guest
webmo
1:00
unlimited
0 jobs

Summary

- CH3ON
- Job # 99922
- 3/12/2012
- 1.7 sec

Actions

-  [Job Manager](#)
-  [Raw output](#)
-  [All files](#)
-  [Print](#)
-  [Help](#)

Notes >>

Molecule Viewer Data Viewer

[Reset Viewer](#)[New Job Using This Geometry](#)[Export Molecule](#)

Calculated Quantities

Quantity	Value																												
Route	#N HF/6-31G(d) SP Geom=Connectivity																												
Stoichiometry	CH ₃ NO																												
Symmetry	C1																												
Basis	6-31G(d)																												
RHF Energy	-168.817822682 Hartree																												
Rotational Constants	<table border="1"> <thead> <tr> <th>Constant</th> <th>Frequency (GHz)</th> <th>Frequency (cm⁻¹)</th> </tr> </thead> <tbody> <tr> <td>a</td> <td>54.5217913</td> <td>1.81865119836</td> </tr> <tr> <td>b</td> <td>10.8831439</td> <td>0.36302260479</td> </tr> <tr> <td>c</td> <td>9.5937326</td> <td>0.32001247343</td> </tr> </tbody> </table>	Constant	Frequency (GHz)	Frequency (cm ⁻¹)	a	54.5217913	1.81865119836	b	10.8831439	0.36302260479	c	9.5937326	0.32001247343																
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Dipole Moment	3.8184 Debye																												
Partial Charges	<table border="1"> <thead> <tr> <th>Atom</th> <th>Symbol</th> <th>Charge</th> <th></th> </tr> </thead> <tbody> <tr> <td>1</td> <td>C</td> <td>0.367643</td> <td></td> </tr> <tr> <td>2</td> <td>N</td> <td>-0.843625</td> <td></td> </tr> <tr> <td>3</td> <td>H</td> <td>0.325638</td> <td></td> </tr> <tr> <td>4</td> <td>H</td> <td>0.372698</td> <td></td> </tr> <tr> <td>5</td> <td>O</td> <td>-0.429048</td> <td></td> </tr> <tr> <td>6</td> <td>H</td> <td>0.206694</td> <td></td> </tr> </tbody> </table>	Atom	Symbol	Charge		1	C	0.367643		2	N	-0.843625		3	H	0.325638		4	H	0.372698		5	O	-0.429048		6	H	0.206694	
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Quote	Everywhere is walking distance if you have the time. -- Steven Wright																												
Server	buchner.chem.hope.edu (26834)																												
CPU time	1.7 sec																												