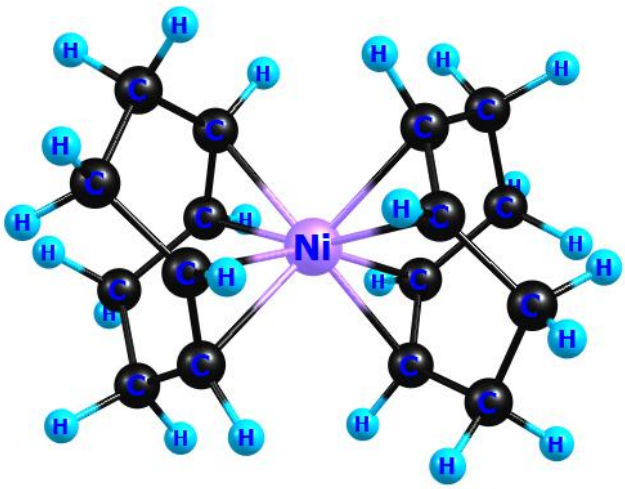
DFT Model Construction and Cartesian Coordinates

The sulfated alumina model applied in this study has been effectively utilized in prior research on similar metal-supported catalysts, demonstrating strong consistency with experimental outcomes.[1-3] The experimental findings from the present work agree well with the predicted structures. A comprehensive description of our model construction was previously provided by Gu et al.[1]

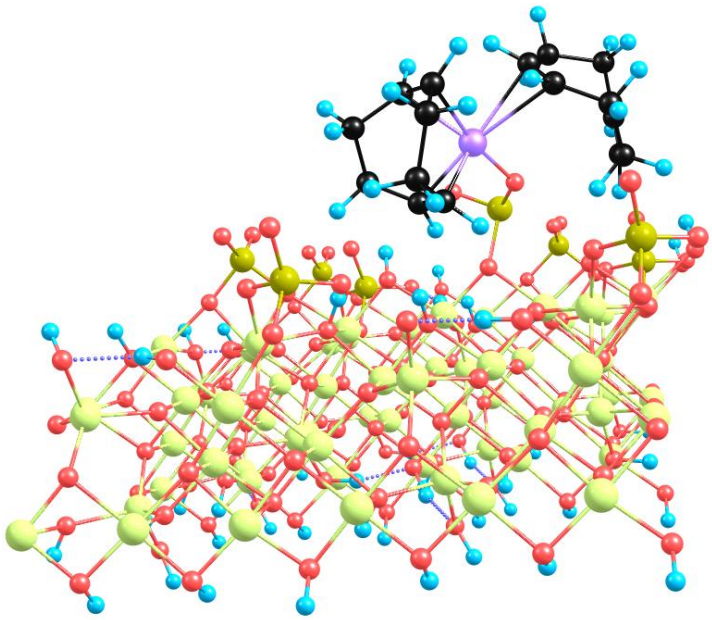
DFT cartesian coordinates (Å) of $Ni(COD)_2$



C	1.867529720	1.186348050	0.477912887
C	2.299569775	-1.676022544	3.238407528
C	3.501676725	-2.588531695	3.360008725
C	4.180423157	-2.873701858	2.002737662
C	4.120690730	-1.676941577	1.064533332
C	3.144782321	-1.455343445	0.089833841
C	1.937077596	-2.333434629	-0.159383265
C	1.256037456	-2.803040463	1.144210004
C	1.226137620	1.249112599	1.717913231
C	1.472637203	2.298497784	2.792391302
C	2.512458968	1.835062727	3.835364950
C	3.604231636	0.973516168	3.237131775
C	4.247439224	1.209169163	2.019467489
C	4.013654744	2.407149330	1.110798243
C	2.970913926	2.112030391	0.011012892
C	1.322719725	-1.750723567	2.241961231
H	1.343019014	0.654602240	-0.321705272
H	0.264958844	0.735594715	1.787710182
H	4.120485306	0.323336449	3.949806002
H	5.202325332	0.699868617	1.874057470

H	5.069022912	-1.154669676	0.922841039
H	3.419589147	-0.801524942	-0.743473253
H	0.377302060	-1.248179948	2.456606177
H	2.028080616	-1.146292079	4.156588404
H	0.523039915	2.518129964	3.302146207
H	1.787292489	3.243198998	2.327886768
H	1.999881617	1.239346774	4.606658581
H	2.945044362	2.705819079	4.363492686
H	4.966333346	2.689494740	0.639181306
H	3.707792276	3.276235491	1.709306626
H	3.478673095	1.627756400	-0.837700455
H	2.550581604	3.055353630	-0.386169141
H	3.226184896	-3.536079211	3.860690601
H	4.229844810	-2.097698061	4.024346833
H	3.725218289	-3.749805806	1.520562748
H	5.233475685	-3.140967468	2.174541265
H	2.207240180	-3.202288359	-0.789019490
H	1.212696747	-1.748852654	-0.747586304
H	1.706128765	-3.740926276	1.497927645
H	0.201525089	-3.037348125	0.936915114
Ni	2.726630483	-0.241992234	1.760353058

DFT cartesian coordinates (Å) of AlS/Ni(COD)$_2$ (1)



Al	1.068509824	5.257117033	8.734515809
Al	5.135981255	7.429364488	7.451484510
O	3.739663152	7.656933556	11.440324621
O	8.023180962	5.312185838	10.011728240

O	3.672519830	7.253406009	8.659500210
O	8.023696208	5.402594169	7.364014694
Al	5.139430877	3.535723886	10.328408672
Al	0.974791183	1.465474356	11.705530256
O	7.945047680	1.282680681	7.608077372
O	3.890443802	3.461331899	8.878029326
O	7.888469026	1.538282201	10.477318245
O	3.762060929	3.329750108	11.505639627
Al	8.092811043	3.473663986	10.306267136
Al	3.811309559	1.440814235	11.491677589
O	5.220934112	1.150815261	7.759724326
O	1.015580680	3.407817389	8.877587143
O	5.352640583	1.618850993	10.473156729
O	0.985612400	3.290530416	11.528816506
Al	3.810158440	5.300766624	8.680302976
Al	8.007715980	7.483272397	7.520342972
O	1.019898047	7.428577685	11.645157775
O	5.151190032	5.349664583	10.145196596
O	1.021075125	7.182802006	8.644123684
O	5.224435530	5.539918217	7.460281061
Al	6.595098321	1.368048689	9.026440779
Al	6.582337870	1.165895089	11.861743143
Al	6.606797774	6.341606214	10.224703209
O	6.609549379	7.433744801	11.672278040
O	6.623330310	7.517001217	8.862906139
Al	2.456410939	7.416781241	10.155032946
Al	2.385434956	7.324348048	7.289938171
Al	2.471251666	2.393447269	8.822949947
O	2.253306392	1.234592544	7.453733822
O	2.329413888	1.229890024	10.307916422
Al	2.364786146	4.377109133	11.546122507
O	2.408370210	5.498189067	10.100751103
O	2.397845206	5.411595092	7.462666152
Al	6.477775309	4.329335343	7.534866782
O	6.620891353	3.286289351	8.988893847
O	6.625193673	3.463016139	11.597410138
H	1.276682755	1.378544791	7.337307489
H	5.239497077	1.753466193	6.996261859
H	7.542037253	1.745437007	6.837221157
H	6.626987345	6.810486130	5.590729516
H	3.846428528	6.566325649	5.637413465
H	0.936611605	8.028413221	5.400963116
H	6.067726285	3.426371980	5.349409733
H	8.569671946	5.203203500	6.574951809
O	6.620950893	7.514367111	6.253741545
O	3.815346130	7.430385016	6.082300841

O	0.934832267	7.341635264	6.083522298
O	6.547067197	3.225813172	6.164118910
Al	9.454069236	5.294697216	8.812120446
Al	13.577760678	7.398811863	7.461190640
O	12.150304980	7.647984057	11.431584134
O	16.436541970	5.246655991	9.926779019
O	12.089103528	7.255843214	8.714679047
O	16.440852875	5.334941781	7.287375379
Al	13.565609511	3.523153730	10.286782269
Al	9.357208090	1.473688255	11.727622376
O	16.360179139	1.222634120	7.599301508
O	12.294613480	3.463368084	8.877154882
O	16.296748354	1.518724643	10.433145060
O	12.224094248	3.323058547	11.516738683
Al	16.531191744	3.427737819	10.220719022
Al	12.242246890	1.440808065	11.485389777
O	13.636836811	1.146312446	7.689677717
O	9.421165392	3.466614029	8.955777636
O	13.765260591	1.593694907	10.417469770
O	9.418232690	3.300277179	11.605437874
Al	12.227791500	5.295318605	8.684268730
Al	16.444572013	7.448084802	7.446723219
O	9.577349812	7.511709996	11.746984531
O	13.616173395	5.326224504	10.084298490
O	9.442631897	7.247862415	8.741657937
O	13.620740653	5.504579474	7.443683249
Al	15.007729076	1.345442185	8.970868243
Al	15.002473718	1.335491240	11.824113156
Al	15.070270983	6.327275094	10.171768120
O	14.879930004	7.427777442	11.601267912
O	15.044623517	7.484046321	8.795713374
Al	10.869718235	7.364835930	10.165499765
Al	10.796418656	7.354091253	7.350012418
Al	10.853953360	2.433602886	8.829559059
O	10.662140874	1.291292521	7.445074904
O	10.746289682	1.281049757	10.315512588
Al	10.815678239	4.360898295	11.600199299
O	10.824290637	5.492923222	10.166690038
O	10.764306926	5.464978425	7.529548196
Al	14.894389053	4.311142843	7.517871692
O	15.031284898	3.236411381	8.956403963
O	15.039552769	3.386880315	11.588016731
H	9.683733825	1.422658892	7.317396114
H	13.707147618	1.749750347	6.927691310
H	15.991914278	1.694046504	6.818303230
H	15.024745466	6.809559616	5.542345298

H	12.222098652	6.685244059	5.610767793
H	9.325433743	8.042632484	5.481510164
H	14.493794757	3.424684943	5.327975497
H	16.961259675	5.113157851	6.488776191
O	15.027883135	7.494268742	6.225560872
O	12.218235794	7.494874932	6.148074617
O	9.342251718	7.353962385	6.162874069
O	14.955884968	3.212996193	6.149670175
Al	1.069054455	13.320914110	8.802255625
Al	5.163287131	15.459046143	7.495631003
O	3.745121993	15.732254536	11.451157719
O	8.023374109	13.387909043	10.066820949
O	3.677984742	15.315521095	8.725248573
O	8.031309526	13.405696731	7.428828503
Al	5.106969205	11.584767710	10.395789156
Al	1.038541767	9.550011923	11.795250646
O	7.942385157	9.348948134	7.676113712
O	3.881249681	11.521480072	8.964808479
O	7.946776716	9.665095167	10.556430117
O	3.824135848	11.451151608	11.674248202
Al	8.036005946	11.567107631	10.283506946
Al	3.750956285	9.506928234	11.807186630
O	5.218594712	9.262291345	7.761997871
O	1.012699596	11.487644009	8.882768357
O	5.373085671	9.676166517	10.561067346
O	0.943806777	11.384864413	11.530256699
Al	3.829864049	13.354974981	8.752708609
Al	8.007432245	15.558722726	7.514834313
O	1.104398737	15.579478888	11.739815822
O	5.210064115	13.388952311	10.152064044
O	1.022456255	15.251246647	8.719676066
O	5.212553282	13.571942169	7.509881328
Al	6.553628597	9.429385776	9.061749294
Al	6.623779566	9.346816375	11.898396631
Al	6.617338408	14.479918932	10.340522822
O	6.389655446	15.555310713	11.673825284
O	6.638721461	15.566438649	8.830359536
Al	2.475060363	15.432751931	10.189324331
Al	2.396520782	15.369624462	7.350432742
Al	2.463839831	10.442258093	8.856002205
O	2.256562213	9.349774489	7.430691496
O	2.336980563	9.285944985	10.250566777
Al	2.356091633	12.410263461	11.617894104
O	2.408259724	13.554240779	10.176443560
O	2.402040498	13.478804274	7.535143214
Al	6.469375768	12.390620767	7.610191400

O	6.622431171	11.309161795	9.036997171
O	6.684034629	11.539219193	11.656795716
H	1.283834241	9.497304898	7.306462985
H	5.297730372	9.877687117	7.009691237
H	7.556754786	9.831082915	6.906454784
H	6.627833778	14.867019887	5.575200518
H	3.845917208	14.637352073	5.681534122
H	0.946066745	16.082270982	5.465791149
H	6.088517272	11.501191681	5.413756679
H	8.560425993	13.183665777	6.634393178
O	6.620851676	15.562951740	6.246837863
O	3.817562584	15.488006682	6.151355642
O	0.937650556	15.402108045	6.154666472
O	6.546450524	11.288696759	6.237890988
Al	9.444388101	13.381356247	8.848298686
Al	13.573217840	15.460671894	7.417552836
O	12.158334132	15.735654257	11.363802337
O	16.429463894	13.320958563	9.994076014
O	12.092994914	15.320527710	8.647308281
O	16.440948152	13.403399500	7.345549180
Al	13.578674155	11.573771629	10.256973106
Al	9.426680950	9.425811102	11.758078518
O	16.359943143	9.293561993	7.589052221
O	12.289661981	11.529923937	8.877438855
O	16.286583942	9.587940210	10.407662446
O	12.230832698	11.385103206	11.504813001
Al	16.533005864	11.480622245	10.221669093
Al	12.258007414	9.483842334	11.477115795
O	13.632674242	9.219822056	7.743906403
O	9.444052112	11.539166087	9.106317785
O	13.747124146	9.621067195	10.410529507
O	9.445407015	11.458653155	11.764720704
Al	12.227773207	13.363499919	8.661813272
Al	16.440168435	15.507433519	7.488855286
O	9.570266275	15.578108912	11.704255852
O	13.567665081	13.395873556	10.087910598
O	9.459047526	15.318729028	8.721338222
O	13.629540401	13.558748451	7.438495096
Al	15.038335986	9.403622817	8.974651291
Al	15.018515787	9.369710410	11.783403385
Al	15.040730118	14.387958768	10.173014231
O	14.885841655	15.499038657	11.604260825
O	15.035195168	15.556230530	8.800094492
Al	10.868258087	15.499310219	10.110806592
Al	10.801798987	15.392093292	7.302050775
Al	10.860000531	10.498070632	8.864593889

O	10.598960293	9.361590605	7.514740608
O	10.742001331	9.352248382	10.347424920
Al	10.972657294	12.559802250	11.586549140
O	10.829916643	13.620755186	10.158813937
O	10.751384512	13.479218391	7.532324182
Al	14.899234116	12.357345927	7.499086118
O	15.025211287	11.307842399	8.951636480
O	15.028771015	11.454568419	11.537947119
H	9.608305653	9.471125063	7.438131415
H	13.694723651	9.804075295	6.966294733
H	15.982630238	9.771525320	6.814724072
H	15.057659908	14.877878059	5.534912270
H	12.237863971	14.653243953	5.584410709
H	9.307689478	16.068991536	5.449885096
H	14.565248389	11.428499686	5.300500868
H	16.999504608	13.190501735	6.568823002
O	15.038181917	15.554747234	6.225640711
O	12.220445355	15.488495848	6.080458341
O	9.338016476	15.408977549	6.157857741
O	14.957018235	11.216718587	6.157948228
O	8.097115026	9.510437170	13.040559771
H	8.192510749	8.981971723	13.858154575
O	12.304106505	10.890398223	14.643360441
H	15.169187121	12.032896369	12.309788628
O	13.450556240	9.445228472	12.962488161
O	11.072034988	9.523720589	12.970938393
S	12.277321453	9.571599455	14.064987527
O	12.300373672	8.395372137	14.881831790
O	-0.466080876	9.442105368	12.958130795
H	-0.315614426	8.910028766	13.761478984
O	1.096758916	15.483053441	14.230704170
O	-0.321989642	13.955098381	12.954623730
O	2.106401533	13.639370458	12.956160431
S	0.969460499	14.656106142	13.049478284
O	9.429368202	15.413229718	14.168743255
O	8.329506980	13.705137676	12.801079647
O	10.743861587	13.723613482	12.943956515
S	9.466361989	14.607494517	12.969418312
H	15.374114743	15.029324398	12.339768673
H	4.666719596	15.365506823	11.540366348
H	12.972912586	15.224632154	11.503616335
O	1.018057158	7.333263788	14.153448853
O	-0.373060367	5.805308624	12.870304678
O	2.096848570	5.561419158	12.876464922
S	0.916371178	6.535193635	12.955315797
O	9.589431857	7.418042477	14.236743353

O	8.172680533	5.879240473	12.962375112
O	10.598067124	5.571672422	12.953157876
S	9.461904680	6.571874302	13.078393327
H	7.122450327	6.933020641	12.373890410
H	4.453724816	7.034310369	11.634055225
H	12.979215445	7.143455713	11.513150402
H	15.356344844	6.941260373	12.337693396
O	8.017589361	1.376151706	13.018924192
H	8.190398174	0.724829604	13.727454343
O	3.666287596	0.492212822	14.958560345
O	12.302559938	0.249768905	14.869264603
O	-0.397045780	1.374088951	12.962590453
H	-0.232093117	0.854651981	13.772044914
O	3.739833991	2.963890348	14.636115523
H	6.734585524	4.029456610	12.381349863
O	4.949178830	1.450325374	13.047250320
O	2.576311168	1.526950604	12.962657958
S	3.724065479	1.634712628	14.081209279
O	12.310414434	2.746096103	14.723093966
H	15.205963011	3.985142135	12.342288283
O	13.459430268	1.370805381	12.965428141
O	11.080192949	1.445129353	13.008746523
S	12.266049447	1.456793970	14.090364055
O	2.393966069	9.525757469	12.883741168
O	5.207544572	9.440879025	13.090071142
O	6.085918631	8.862931613	15.359361713
S	4.775942427	9.078914881	14.708219454
H	8.959988511	11.812613159	12.546106713
O	4.140741614	10.424975111	15.211377310
H	6.680109625	12.243006604	12.330463742
C	5.594345056	13.532043632	17.374838669
C	3.377969577	11.453102790	18.039614752
C	2.946843427	10.102986005	18.540163639
C	1.503364641	9.658751820	18.235808829
C	1.373112315	9.178014741	16.817879901
C	1.297903662	9.901599322	15.693258438
C	1.203680939	11.365144503	15.432829716
C	1.396255271	12.359136694	16.585730246
C	6.567551261	12.555299730	17.474797631
C	7.895887442	12.608351194	16.762943669
C	7.857364326	11.769424070	15.478706662
C	6.531046769	11.848752826	14.780583472
C	5.700144602	12.968458175	14.607349165
C	6.044540839	14.378008833	15.012480239
C	5.591146945	14.714268031	16.449220149
C	2.738953681	12.382336204	17.261481943

H	4.863064617	13.578247703	18.184504152
H	6.479312355	11.831267992	18.293100785
H	6.327391722	11.008433522	14.124046460
H	4.867189376	12.839789246	13.903969026
H	1.475491499	8.097625715	16.678892164
H	1.404305267	9.345088228	14.765113458
H	3.206090071	13.368543331	17.222747315
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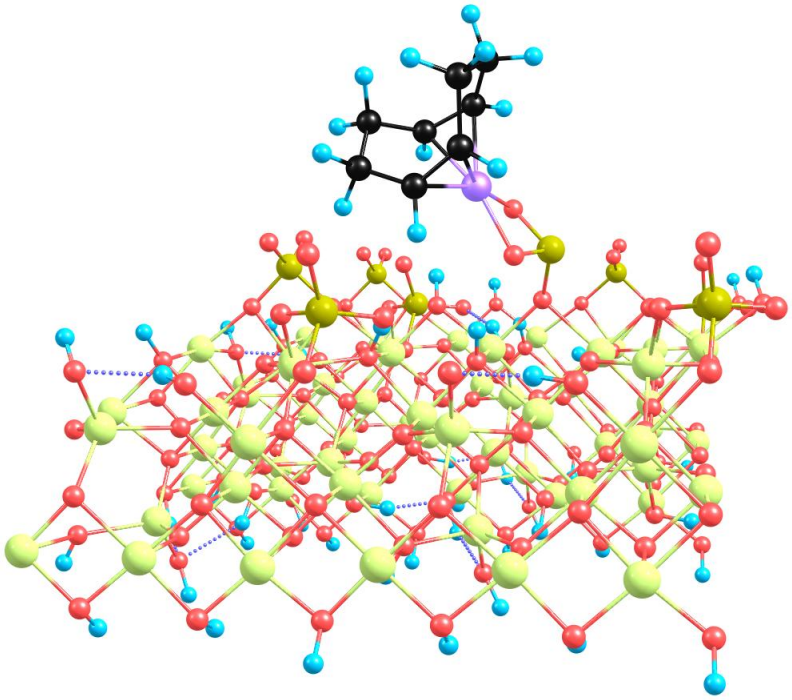
DFT cartesian coordinates (Å) of AlS/Ni(COD)



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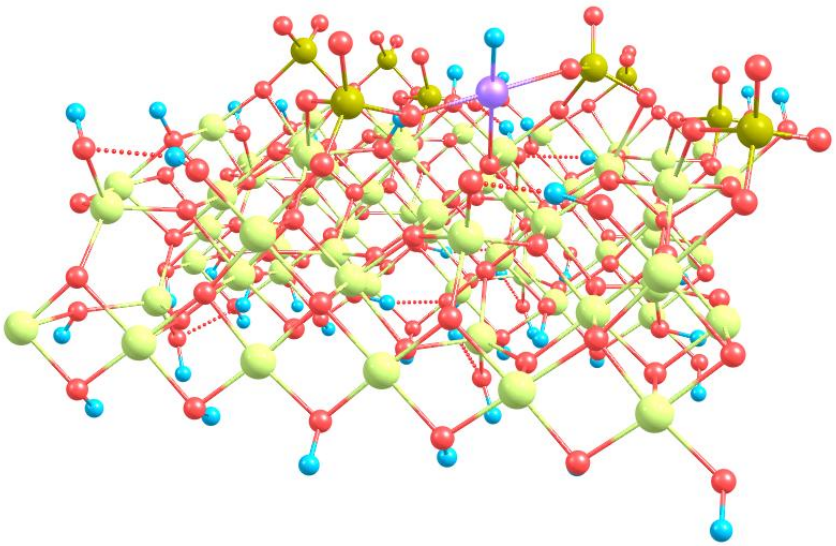

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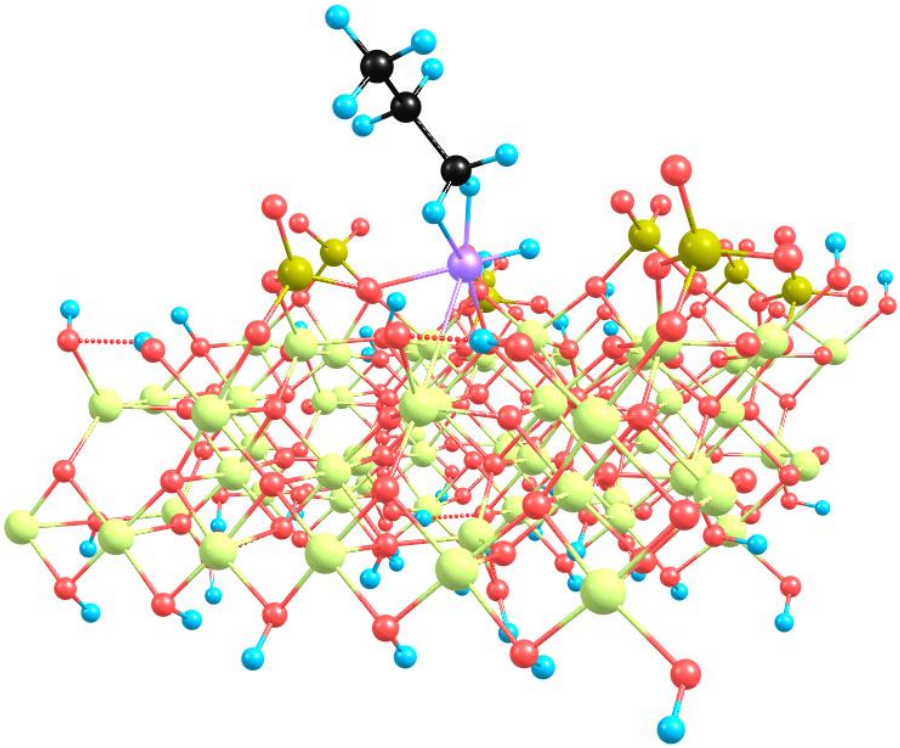

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C	6.351575691	15.531568662	16.070616745
H	5.291384387	15.663425434	16.320083366
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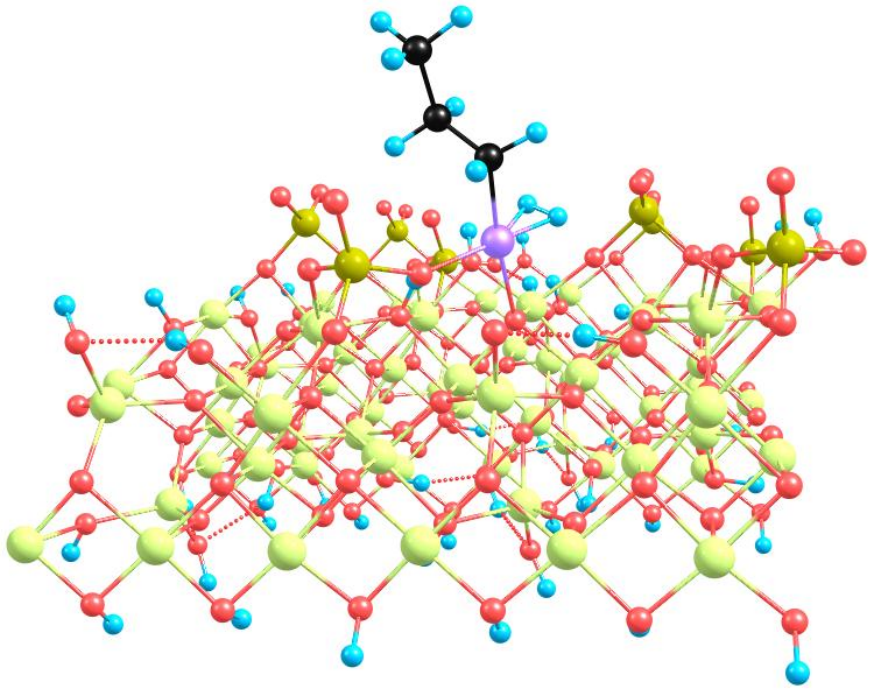

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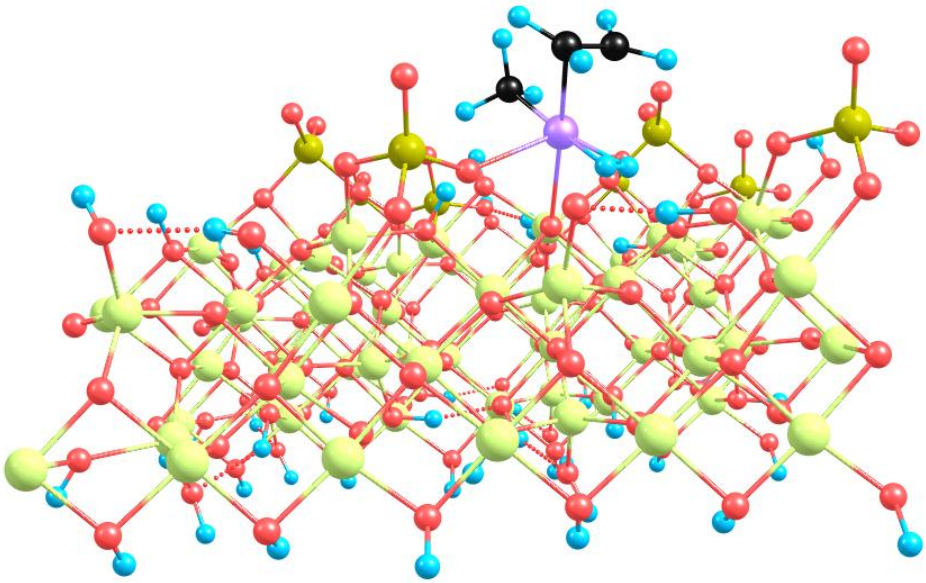
DFT cartesian coordinates (Å) of INT4



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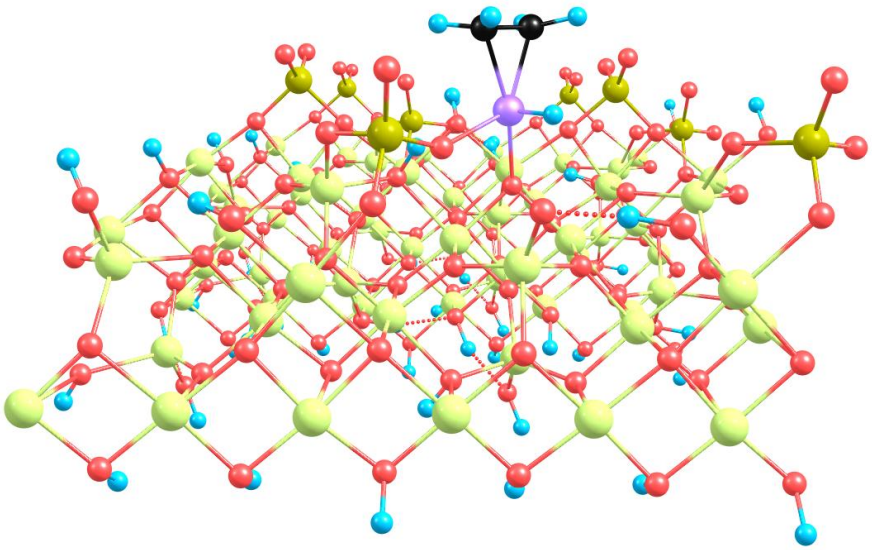
DFT cartesian coordinates (Å) of INT5



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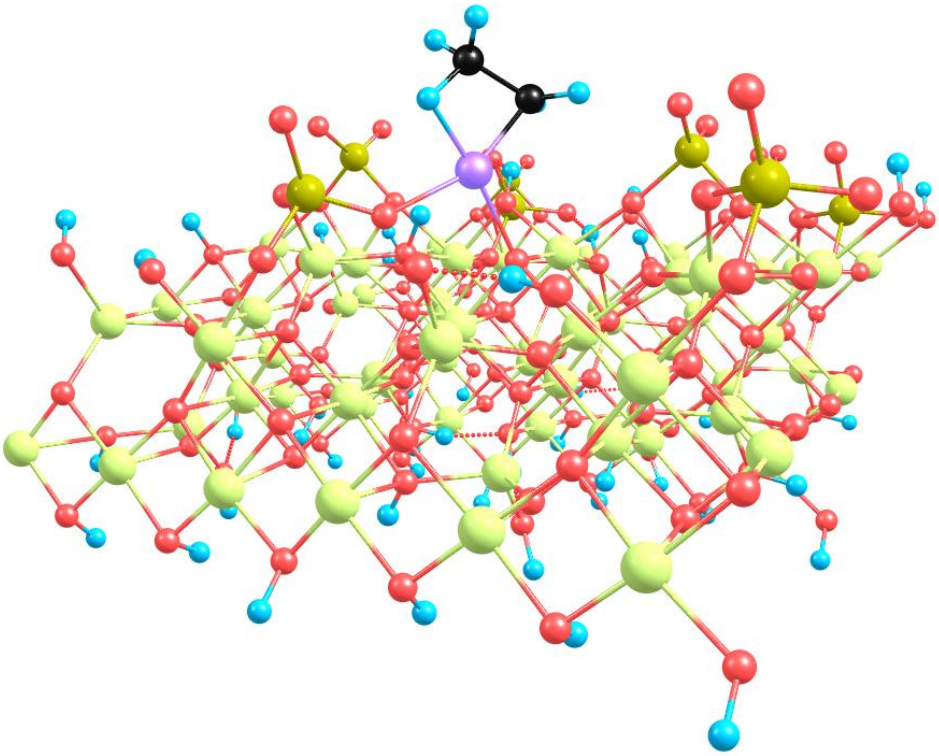

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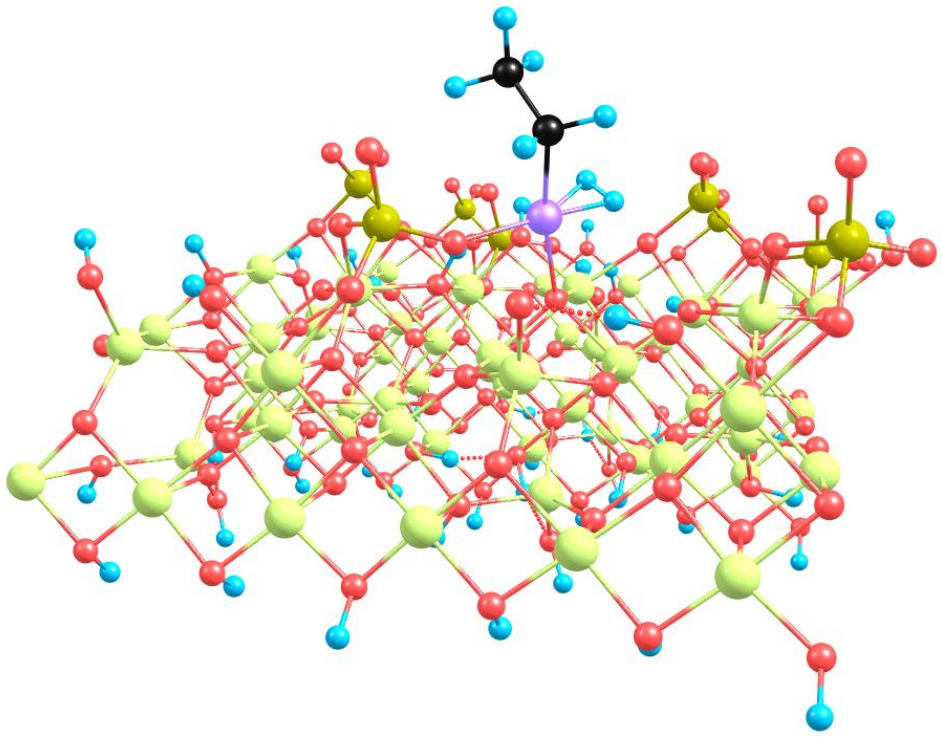

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C	7.145114871	13.054681509	15.734164357
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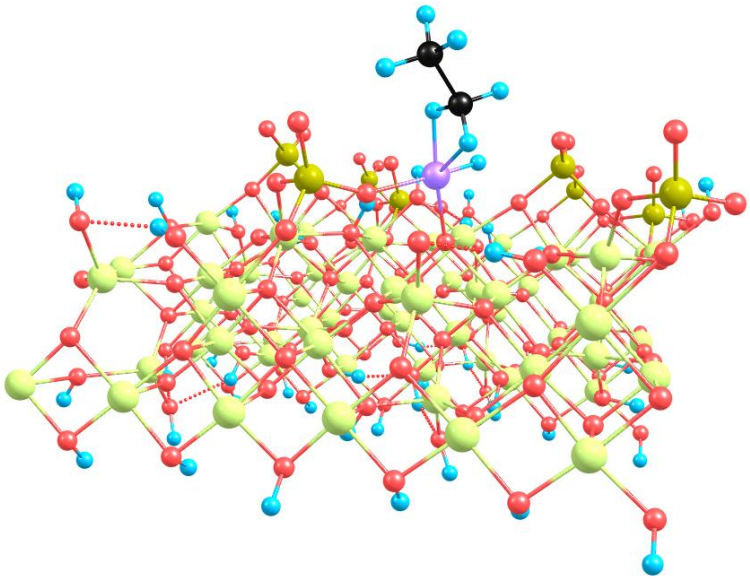
DFT cartesian coordinates (Å) of INT8



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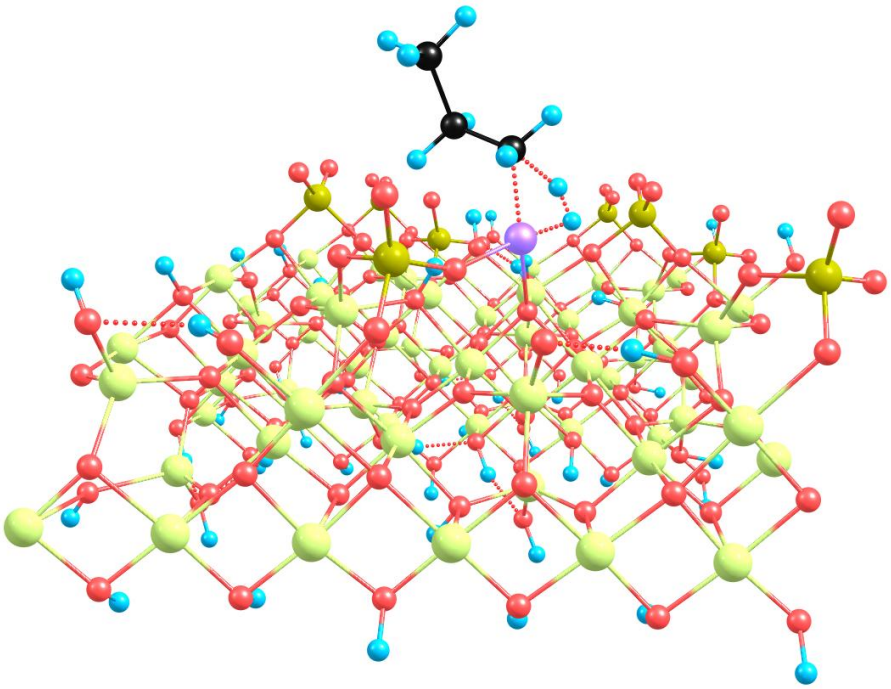

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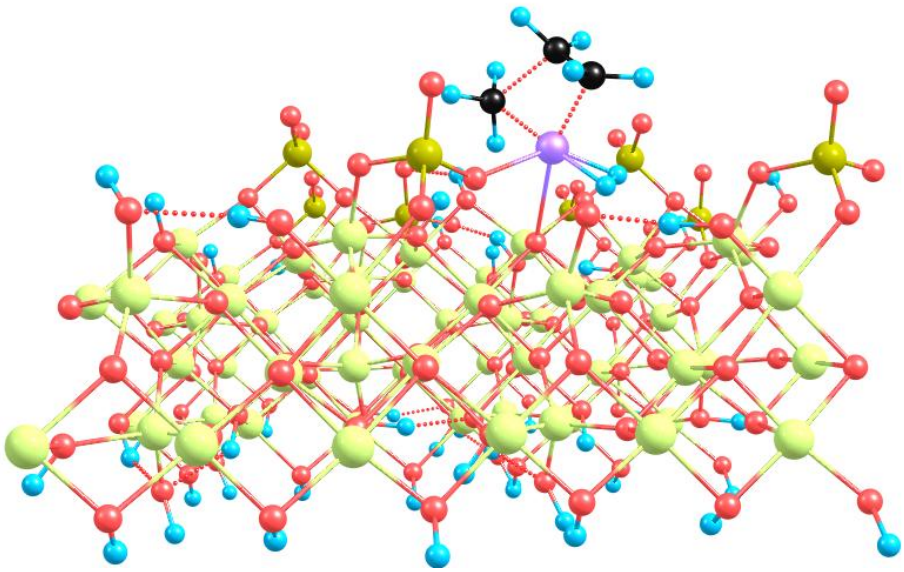
DFT cartesian coordinates (Å) of TS2



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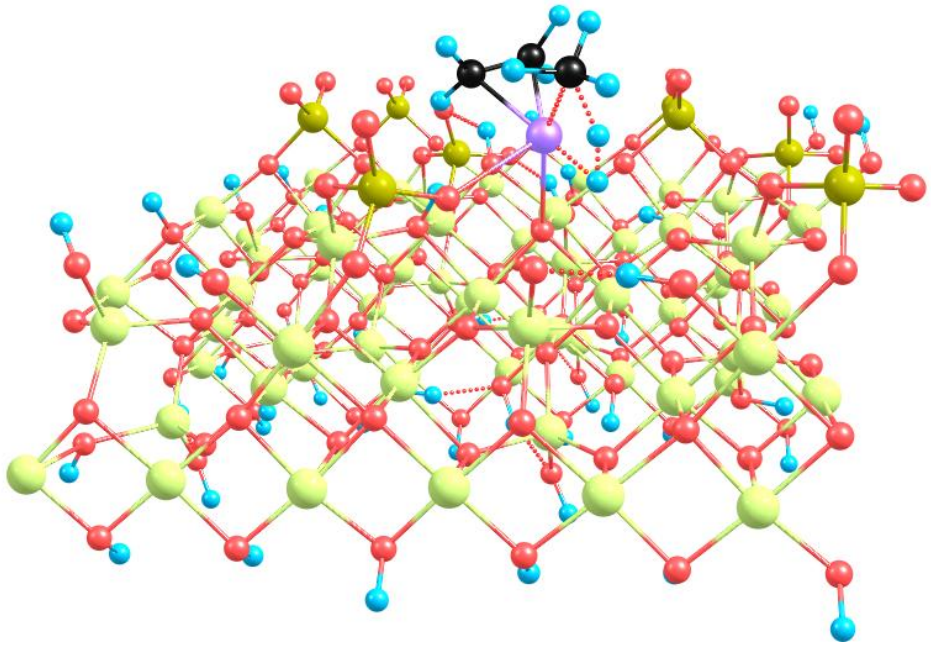
DFT cartesian coordinates (Å) of TS3



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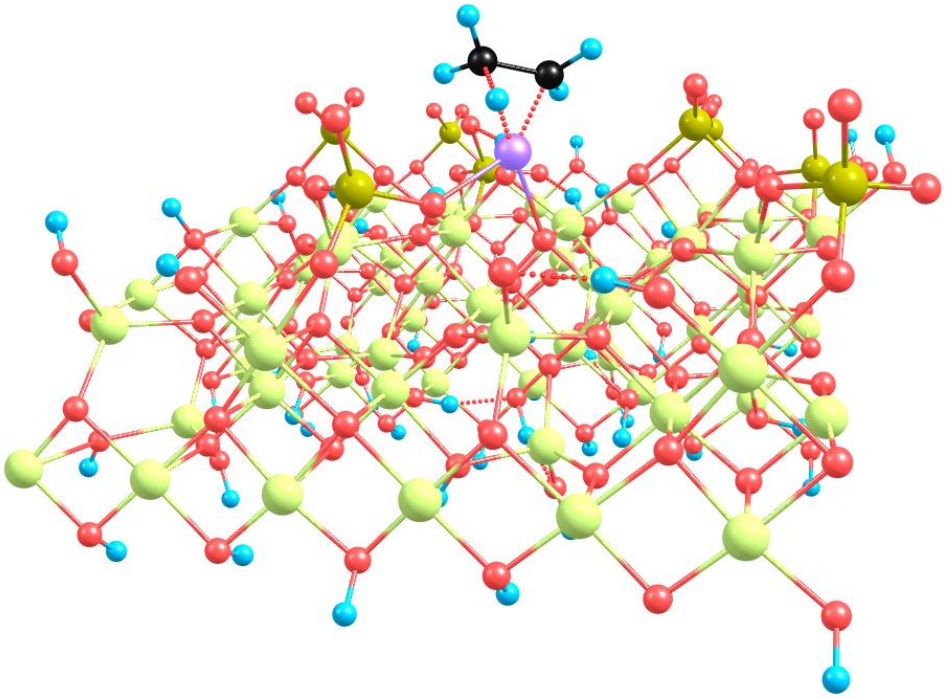
DFT cartesian coordinates (Å) of TS4



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C	7.637534985	11.561302677	14.991222899
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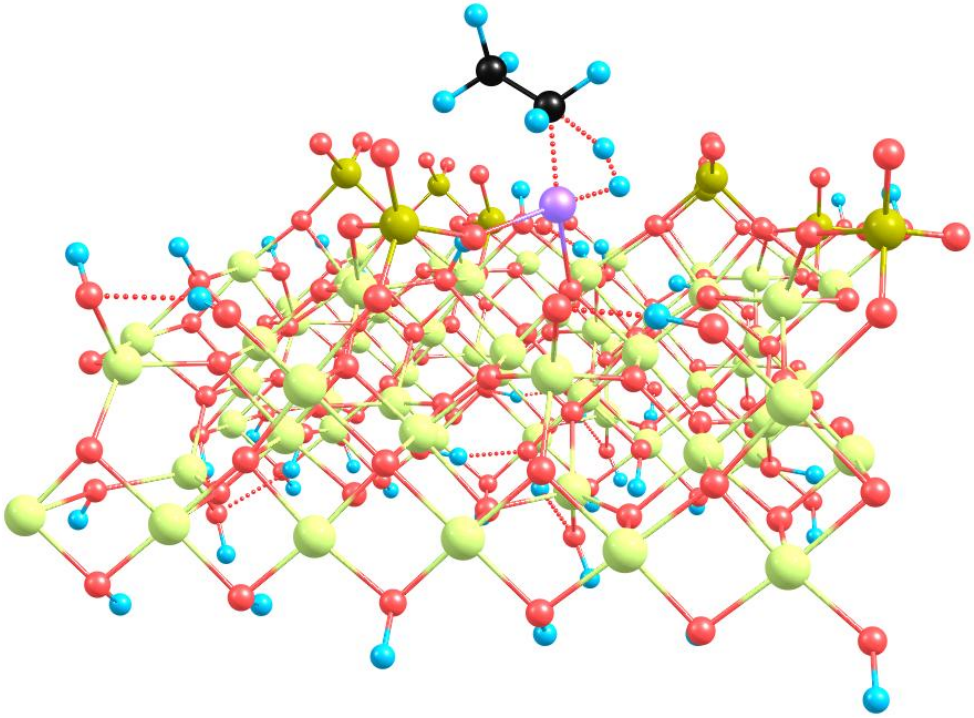
DFT cartesian coordinates (Å) of TS5



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C	7.829950724	12.434314994	15.575964574
H	7.994418785	13.042085671	16.482116494
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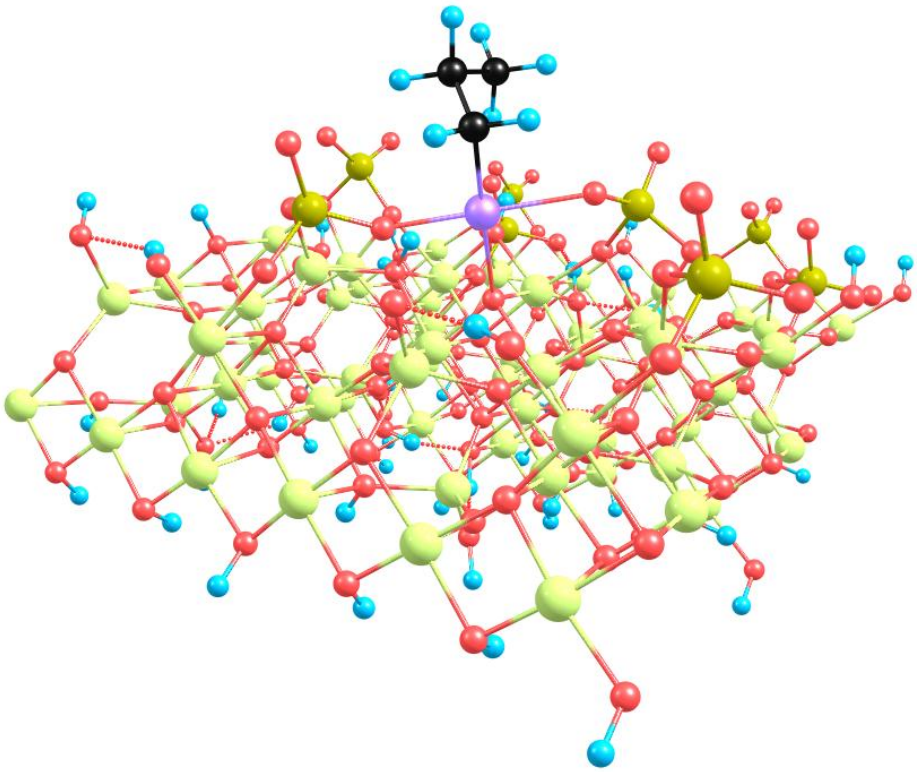
DFT cartesian coordinates (Å) of INT3b



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Al	4.851723484	3.262388589	9.923710965
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Al	7.777912738	3.166405827	9.912882467
Al	3.526789714	1.177433599	11.104201566
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Al	6.310018420	6.054908774	9.806719110
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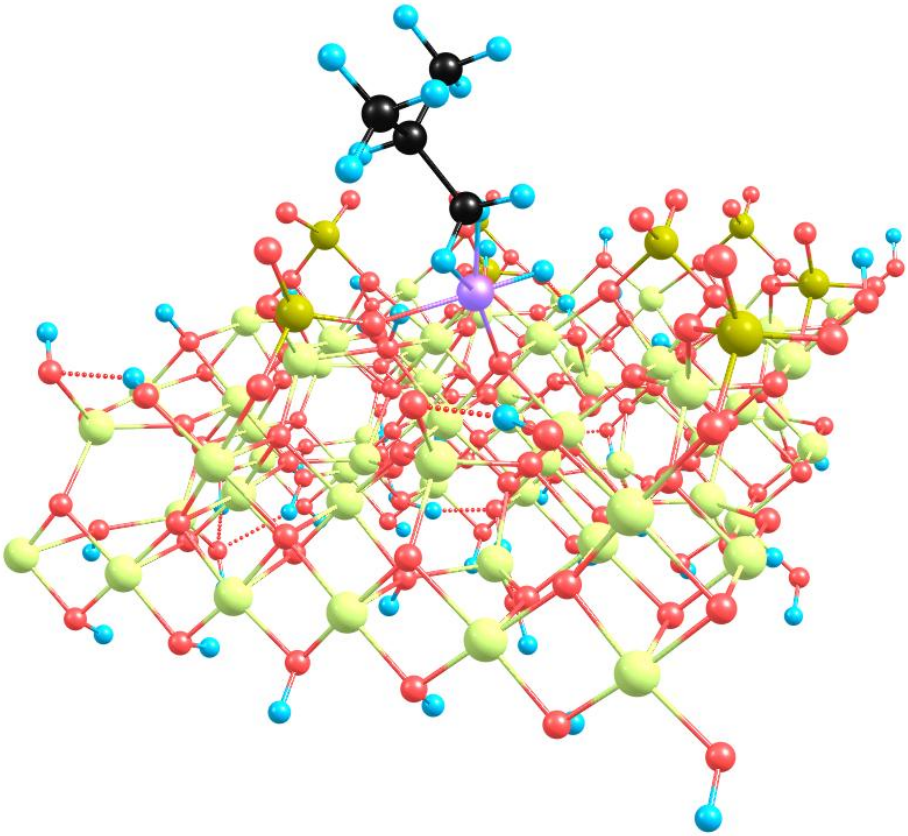
DFT cartesian coordinates (Å) of INT2-ISO



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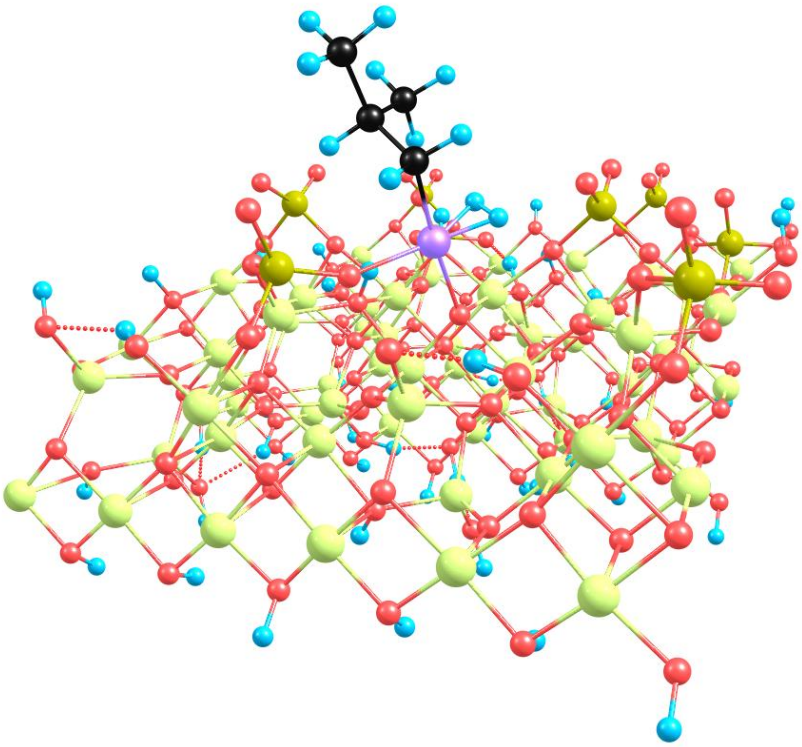

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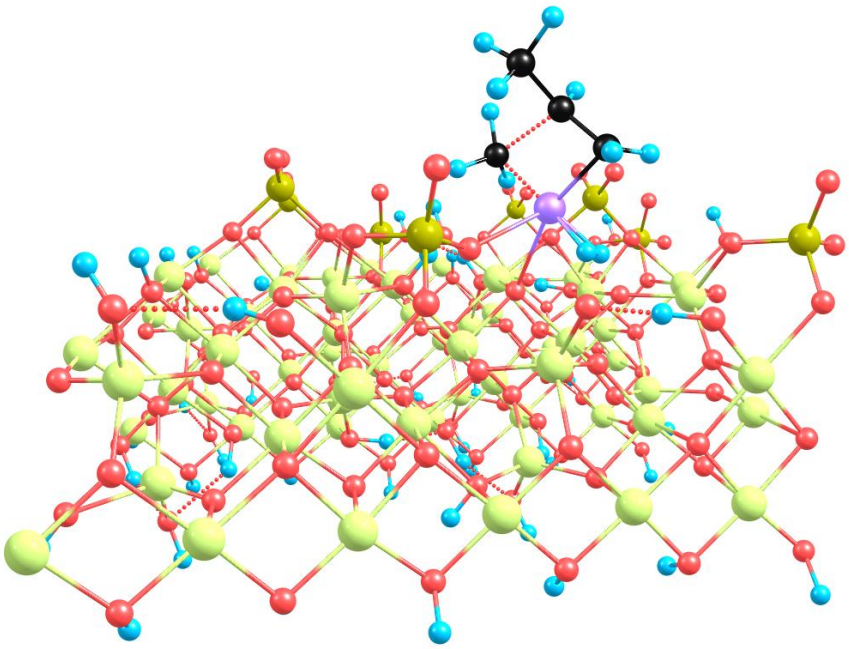

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O	4.848227240	5.078370661	9.692003262
O	0.706587571	6.933639207	8.326479431
O	4.899925499	5.232838100	7.045389212
Al	6.277704904	1.067123153	8.649020102
Al	6.270676989	0.869307169	11.483598808
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O	6.229497738	7.179134390	11.262306640
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Al	2.077886748	4.080106248	11.188202837
O	2.087602544	5.218616963	9.761122231
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Al	6.156878626	4.021773446	7.128074188
O	6.311450212	2.983069835	8.581700349
O	6.319759084	3.212904235	11.189511989
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H	7.260321041	1.415198667	6.486407270
H	6.301881437	6.487065155	5.174790094
H	3.512320730	6.357664133	5.229884480
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O	6.306363417	7.188268476	5.840344680
O	3.493450253	7.180606339	5.746146422
O	0.621666955	7.031235530	5.752289192
O	6.235324167	2.904003384	5.767030552
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Al	11.935860403	1.177404916	11.139117120
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O	13.466512829	1.300564237	10.074228194
O	9.108179244	2.986842277	11.203437337
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O	9.268197126	7.185664944	11.344034654
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O	9.126734147	6.933772103	8.332510587
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Al	14.578552058	4.025812511	7.121050365
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H	4.969006343	9.555930152	6.597300045
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O	15.994769099	9.283840251	10.086600331
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O	10.812312916	9.202441425	12.647247343
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O	-0.696668385	9.122514284	12.631276336
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O	0.859959884	15.175379404	13.845337432
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O	1.798810491	13.321943574	12.557111567
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O	9.273050489	7.096386624	13.835608326
O	7.852102828	5.559544408	12.559220848
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H	6.694509021	6.700116172	11.995986634
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H	15.160487613	6.631171300	11.970780819
O	7.702789996	1.121854536	12.631149748
H	7.858890943	0.500789124	13.370192680
O	3.499128306	0.165693833	14.562787593
O	11.989096301	-0.078577360	14.469985245
O	-0.703562791	1.124047044	12.625547375
H	-0.565004463	0.630820622	13.454639385
O	3.504706561	2.647603621	14.238518142
H	6.446319401	3.779042206	11.970850103
O	4.692775588	1.140499717	12.633017185
O	2.330888307	1.209783059	12.578269549
S	3.497838500	1.312897027	13.699543162
O	11.997755144	2.416855911	14.465220235
H	14.856649329	3.722121252	11.971293334
O	13.159107121	1.132616120	12.632321029
O	10.785490367	1.206782878	12.651732371
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O	3.582194589	10.565037883	14.322534915
O	2.370628591	9.198407460	12.642658809
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O	3.577502489	8.076399081	14.557067264
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Ni	5.916103495	12.345751203	13.280479647
H	8.579419184	11.458660423	12.179461506
C	5.089429728	13.551730733	14.530768831
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C	5.863557579	12.747476467	15.419221349
H	5.272464680	12.019342980	15.980032135
C	6.902582599	11.181555211	14.551345281
H	7.909370283	11.407199201	14.171562857
H	6.402321990	10.349804579	14.040719799
H	7.003866028	10.890057084	15.596252706
H	5.452634765	13.510189951	12.311303192
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C	7.004593530	13.394272281	16.173017659
H	6.573735552	14.081525649	16.916414993

H	7.627403758	12.665820777	16.706917048
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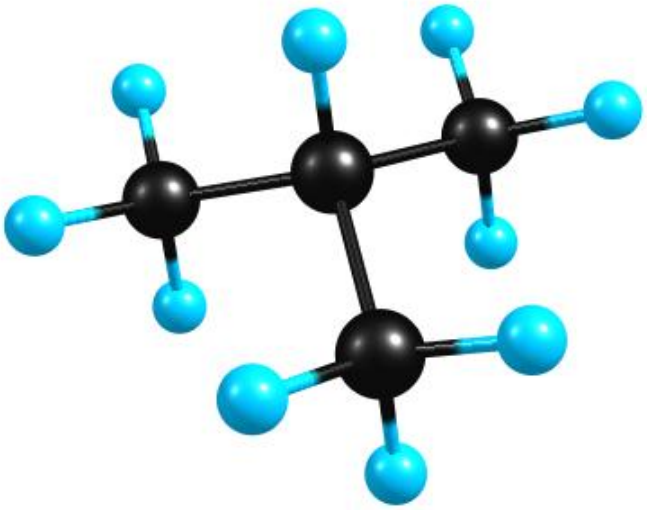
DFT cartesian coordinates (Å) of Isobutane



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H	6.192639451	12.465947702	15.664276004
H	6.791715884	14.049317309	16.203008763
C	4.109956863	14.286184804	15.445720820
H	3.280296799	14.764754740	14.905541590
H	3.764921943	13.301198981	15.792646252
H	4.322775589	14.897292441	16.337102892
H	5.097932788	13.545738452	13.688296767
C	5.804015723	15.541235746	14.054023759
H	6.075607722	16.197301656	14.896011287
H	6.682053061	15.462046002	13.396688713
H	5.002639139	16.040130489	13.489670060
H	7.386204257	13.347343101	14.683511085

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