Supporting Information

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Interplay Between Site Activity and Density of BCC Iron for Ammonia Synthesis Based on First-Principles Theory

Bing-Yan Zhang[+], Hai-Yan Su[+], Jin-Xun Liu, and Wei-Xue Li*

Supporting Information

Interplay Between Site Activity and Density of BCC Iron for Ammonia Synthesis Based on First-Principles Theory

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Chinese Academy of Sciences.
Dalian 116023, China.

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Chinese Academy of Sciences.
Dalian 116023, China.

[c] Dr. Jin-Xun, Liu
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University of Michigan.
Ann Arbor, MI 48109-2136, USA

[d] Pro, Dr. Wei-Xue, Li
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University of Science and Technology of China
Hefei 230026, China
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[e] Bing-Yan, Zhang#
University of Chinese Academy of Sciences
Chinese Academy of Sciences
Beijing 100049, China

# These authors contribute equally to this work

Structure of Adsorption Structure and Transition States

1. (100) surface

1.1 H adsorption.cif

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_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 5.6640

_cell_length_b 5.6640

_cell_length_c 24.9120

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.7628	0.7042	0.0000
Fe	Fe3	0.2628	0.2042	0.0000
Fe	Fe4	0.7628	0.2042	0.0000
Fe	Fe5	0.5128	0.4542	0.0568
Fe	Fe6	0.0128	0.4542	0.0568
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Fe	Fe9	0.2628	0.2042	0.1137
Fe	Fe10	0.7628	0.2042	0.1137
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Fe	Fe12	0.2628	0.7042	0.1137

Fe	Fe13	0.0128	0.4542	0.1705
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Fe	Fe15	0.5128	0.4542	0.1705
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Fe	Fe17	0.2628	0.2042	0.2274
Fe	Fe18	0.7628	0.2042	0.2274
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Fe	Fe32	0.0083853809530454	0.4492607516867807	0.4005643157370247
H	H33	0.2641353742949291	0.7029227747732213	0.4158431661500854

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_cell_length_c 24.9120

_cell_angle_alpha 90.0000

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loop_

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_atom_site_label

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Fe	Fe12	0.2628	0.7042	0.1137
Fe	Fe13	0.0128	0.4542	0.1705
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Fe Fe25 0.7629 0.2042 0.3459

Fe Fe26 0.2630 0.7042 0.3372

Fe Fe27 0.7629 0.7042 0.3436

Fe Fe28 0.2629 0.2042 0.3436

Fe Fe29 0.5020 0.9433 0.4003

Fe Fe30 0.5018 0.4653 0.4002

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1.3 N_2 adsorption.cif

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loop_

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Fe Fe2 0.7628 0.7042 0.0000

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Fe	Fe4	0.7628	0.2042	0.0000
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loop_
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1.5 NH_2 adsorption.cif

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_cell_angle_alpha 90.0000

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_atom_site_label

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_atom_site_fract_y

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Fe	Fe28	0.2697569920318562	0.2042400560585456	0.3440198083365987
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Fe	Fe32	0.0133365998384302	0.4456323108921921	0.3967141235152499
N	N33	0.5127675190825886	0.7043641396406254	0.4647575324376336
H	H34	0.3662510854675686	0.7041425717013630	0.4889122638003949
H	H35	0.6589716246059285	0.7041008891517051	0.4890088188842059

1.6 NH_3 adsorption.cif

data_

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_cell_length_b 5.6640
_cell_length_c 24.9120
_cell_angle_alpha 90.0000
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_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

Fe	Fe1	0.2628	0.7042	0.0000
Fe	Fe2	0.7628	0.7042	0.0000

Fe	Fe3	0.2628	0.2042	0.0000
Fe	Fe4	0.7628	0.2042	0.0000
Fe	Fe5	0.5128	0.4542	0.0568
Fe	Fe6	0.0128	0.4542	0.0568
Fe	Fe7	0.0128	0.9542	0.0568
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Fe	Fe25	0.7614957259724795	0.2054465862362970	0.3439516487733801
Fe	Fe26	0.2642006800997154	0.7027823859648137	0.3438425268165431
Fe	Fe27	0.7615502169802764	0.7027382125130417	0.3438389179681718
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H	H35	0.3661677835384932	0.5439722836593168	0.5052090591420955

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1.7 N_2 activation.cif

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Fe Fe3 0.2628 0.2042 0.0000
Fe Fe4 0.7628 0.2042 0.0000
Fe Fe5 0.5128 0.4542 0.0568
Fe Fe6 0.0128 0.4542 0.0568
Fe Fe7 0.0128 0.9542 0.0568
Fe Fe8 0.5128 0.9542 0.0568
Fe Fe9 0.2628 0.2042 0.1137
Fe Fe10 0.7628 0.2042 0.1137
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Fe	Fe18	0.7628	0.2042	0.2274
Fe	Fe19	0.7628	0.7042	0.2274
Fe	Fe20	0.2628	0.7042	0.2274
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Fe	Fe32	-0.0210	0.4221	0.4012
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1.8 N+H hydrogenation.cif

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Fe	Fe18	0.7628	0.2042	0.2274
Fe	Fe19	0.7628	0.7042	0.2274
Fe	Fe20	0.2628	0.7042	0.2274
Fe	Fe21	0.0101625159494360	0.9566588132667353	0.2850721526460049
Fe	Fe22	0.0101871417212092	0.4516602439400705	0.2850744741339380

Fe	Fe23	0.5157413700059835	0.9576037634722380	0.2851388719037161
Fe	Fe24	0.5157919560203680	0.4506689807161659	0.2851494615370099
Fe	Fe25	0.7627568620862530	0.2041260749215793	0.3459070398083994
Fe	Fe26	0.2648486302107252	0.7041151739519735	0.3384041515641676
Fe	Fe27	0.7627863166350402	0.7041044059785551	0.3436291232874317
Fe	Fe28	0.2609999476591680	0.2041071926002546	0.3434706677290219
Fe	Fe29	0.5084033526211437	0.9532177745437871	0.4007426753485460
Fe	Fe30	0.5083490443113378	0.4550194132828185	0.4007343429843250
Fe	Fe31	0.0218578292793263	0.9482541944315349	0.3998912054209555
Fe	Fe32	0.0216838008439904	0.4600025087196877	0.3999084590994665
N	N33	0.2522873623184319	0.7040757991262775	0.4175738816150667
H	H34	0.4721906952676402	0.7041227607456905	0.4433102634008517

1.9 HN+H hydrogenation.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 5.6640
_cell_length_b 5.6640
_cell_length_c 24.9120
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

Fe	Fe1	0.2628	0.7042	0.0000
Fe	Fe2	0.7628	0.7042	0.0000
Fe	Fe3	0.2628	0.2042	0.0000
Fe	Fe4	0.7628	0.2042	0.0000
Fe	Fe5	0.5128	0.4542	0.0568
Fe	Fe6	0.0128	0.4542	0.0568
Fe	Fe7	0.0128	0.9542	0.0568
Fe	Fe8	0.5128	0.9542	0.0568
Fe	Fe9	0.2628	0.2042	0.1137
Fe	Fe10	0.7628	0.2042	0.1137
Fe	Fe11	0.7628	0.7042	0.1137
Fe	Fe12	0.2628	0.7042	0.1137
Fe	Fe13	0.0128	0.4542	0.1705
Fe	Fe14	0.5128	0.9542	0.1705
Fe	Fe15	0.5128	0.4542	0.1705
Fe	Fe16	0.0128	0.9542	0.1705
Fe	Fe17	0.2628	0.2042	0.2274
Fe	Fe18	0.7628	0.2042	0.2274
Fe	Fe19	0.7628	0.7042	0.2274
Fe	Fe20	0.2628	0.7042	0.2274
Fe	Fe21	0.0095227965628307	0.9589655375949243	0.2853738304306525
Fe	Fe22	0.0094758172106128	0.4494635822935189	0.2853679145237423
Fe	Fe23	0.5174870919148891	0.9594824832111986	0.2853785137362932
Fe	Fe24	0.5175052117717543	0.4489508939183497	0.2853725364964845
Fe	Fe25	0.7628141559541118	0.2041915346040268	0.3467727384583536
Fe	Fe26	0.2632799871520461	0.7041562158550385	0.3376959080478638
Fe	Fe27	0.7627052258687812	0.7042784711375293	0.3433394626138553
Fe	Fe28	0.2639669685275466	0.2042731742847388	0.3443548866505762
Fe	Fe29	0.5028850769496332	0.9427380299029712	0.4014804477669853
Fe	Fe30	0.5024352007767966	0.4663435492934143	0.4015087202155848
Fe	Fe31	0.0213868986866204	0.9389220375141971	0.4008846120378484
Fe	Fe32	0.0202507850982529	0.4690556390152397	0.4008378841064264
N	N33	0.3261466524365418	0.7047668936056957	0.4438971454973862

H H34 0.0628106662806349 0.7040788723019298 0.4454320890289254

H H35 0.3449358959148854 0.7049014434741564 0.4852583287605591

1.10 H_2N+H hydrogenation.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 5.6640

_cell_length_b 5.6640

_cell_length_c 24.9120

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe Fe1 0.2628 0.7042 0.0000

Fe Fe2 0.7628 0.7042 0.0000

Fe Fe3 0.2628 0.2042 0.0000

Fe Fe4 0.7628 0.2042 0.0000

Fe Fe5 0.5128 0.4542 0.0568

Fe Fe6 0.0128 0.4542 0.0568

Fe Fe7 0.0128 0.9542 0.0568

Fe Fe8 0.5128 0.9542 0.0568

Fe Fe9 0.2628 0.2042 0.1137

Fe Fe10 0.7628 0.2042 0.1137

Fe	Fe11	0.7628	0.7042	0.1137
Fe	Fe12	0.2628	0.7042	0.1137
Fe	Fe13	0.0128	0.4542	0.1705
Fe	Fe14	0.5128	0.9542	0.1705
Fe	Fe15	0.5128	0.4542	0.1705
Fe	Fe16	0.0128	0.9542	0.1705
Fe	Fe17	0.2628	0.2042	0.2274
Fe	Fe18	0.7628	0.2042	0.2274
Fe	Fe19	0.7628	0.7042	0.2274
Fe	Fe20	0.2628	0.7042	0.2274
Fe	Fe21	0.0125034810909162	0.9555465782155641	0.2851430767084364
Fe	Fe22	0.0110829546571438	0.4524770621245359	0.2850588107296976
Fe	Fe23	0.5130192945471331	0.9538378656580675	0.2851917528600637
Fe	Fe24	0.5156702038364145	0.4542926730293342	0.2851176711023013
Fe	Fe25	0.7600725061493120	0.2007837051731389	0.3438682698856404
Fe	Fe26	0.2618142360663994	0.7012233018585408	0.3418859157154778
Fe	Fe27	0.7634061854196514	0.7074041759197168	0.3433114099323497
Fe	Fe28	0.2681575069476415	0.2059674998333617	0.3428554873317410
Fe	Fe29	0.4936913467492737	0.9523810561033272	0.4014592090497467
Fe	Fe30	0.5233852456662583	0.4640027627320402	0.4033716889137172
Fe	Fe31	0.0305971552726246	0.9588869709090003	0.4000786451337837
Fe	Fe32	0.0044825701487773	0.4425023534601297	0.3967717863963684
N	N33	0.4643541125140976	0.6777226406973134	0.4687699695696937
H	H34	0.3189941730719272	0.8615355795758078	0.4531490342821100
H	H35	0.3332203129499405	0.6097504670362872	0.4927657366368262
H	H36	0.6015543675823325	0.7259354296171175	0.4935260532986929

2. (110) surface

2.1 H adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 4.9052

_cell_length_b 4.9052

_cell_length_c 25.0126

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 70.5287

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.1978	0.2894	0.0000
Fe	Fe2	0.6978	0.2894	0.0000
Fe	Fe3	0.1978	0.7894	0.0000
Fe	Fe4	0.6978	0.7894	0.0000
Fe	Fe5	0.4478	0.0394	0.0801
Fe	Fe6	0.4478	0.5394	0.0801
Fe	Fe7	0.9478	0.5394	0.0801
Fe	Fe8	0.9478	0.0394	0.0801
Fe	Fe9	0.1978	0.7894	0.1601
Fe	Fe10	0.6978	0.2894	0.1601
Fe	Fe11	0.6978	0.7894	0.1601
Fe	Fe12	0.1978	0.2894	0.1601
Fe	Fe13	0.9470179302229980	0.0393346996967506	0.2400089659429324
Fe	Fe14	0.4463687640605379	0.5399693144518611	0.2400055573157164
Fe	Fe15	0.9466022370719813	0.5395859167981547	0.2401131498965484
Fe	Fe16	0.4467684931469324	0.0397327761141059	0.2400391780168057
Fe	Fe17	0.1960058091762910	0.2898269723354152	0.3207475860100096

Fe Fe18 0.6958246808686384 0.2898920452740718 0.3205574399068368

Fe Fe19 0.1955287597718844 0.7896060778651245 0.3211845585112705

Fe Fe20 0.6957505686905987 0.7901070509143830 0.3207531680341962

Fe Fe21 0.4441625911400687 0.5424277281334350 0.4010790739399581

Fe Fe22 0.9466788868846313 0.5412545454207713 0.4009826536421896

Fe Fe23 0.4445275050207392 0.0392156589650968 0.4010256782533629

Fe Fe24 0.9478129505119418 0.0388016812808238 0.4010769796095908

H H25 0.7563750890140233 0.3509753280227042 0.4392422434174774

2.2 N adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 4.9052

_cell_length_b 4.9052

_cell_length_c 25.0126

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 70.5287

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe Fe1 0.1978 0.2894 0.0000

Fe Fe2 0.6978 0.2894 0.0000

Fe Fe3 0.1978 0.7894 0.0000

Fe Fe4 0.6978 0.7894 0.0000

Fe	Fe5	0.4478	0.0394	0.0801
Fe	Fe6	0.4478	0.5394	0.0801
Fe	Fe7	0.9478	0.5394	0.0801
Fe	Fe8	0.9478	0.0394	0.0801
Fe	Fe9	0.1978	0.7894	0.1601
Fe	Fe10	0.6978	0.2894	0.1601
Fe	Fe11	0.6978	0.7894	0.1601
Fe	Fe12	0.1978	0.2894	0.1601
Fe	Fe13	0.9463	0.0402	0.2400
Fe	Fe14	0.4475	0.5390	0.2400
Fe	Fe15	0.9470	0.5397	0.2403
Fe	Fe16	0.4467	0.0394	0.2403
Fe	Fe17	0.1961	0.2896	0.3221
Fe	Fe18	0.6961	0.2896	0.3202
Fe	Fe19	0.1962	0.7896	0.3190
Fe	Fe20	0.6961	0.7895	0.3221
Fe	Fe21	0.4077	0.5774	0.4002
Fe	Fe22	0.9292	0.5233	0.4032
Fe	Fe23	0.4621	0.0559	0.4031
Fe	Fe24	0.9836	0.0017	0.4002
N	N25	0.6956	0.2896	0.4292

2.3 N_2 adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 4.9052

_cell_length_b 4.9052

_cell_length_c 25.0126

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 70.5287

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.1978	0.2894	0.0000
Fe	Fe2	0.6978	0.2894	0.0000
Fe	Fe3	0.1978	0.7894	0.0000
Fe	Fe4	0.6978	0.7894	0.0000
Fe	Fe5	0.4478	0.0394	0.0801
Fe	Fe6	0.4478	0.5394	0.0801
Fe	Fe7	0.9478	0.5394	0.0801
Fe	Fe8	0.9478	0.0394	0.0801
Fe	Fe9	0.1978	0.7894	0.1601
Fe	Fe10	0.6978	0.2894	0.1601
Fe	Fe11	0.6978	0.7894	0.1601
Fe	Fe12	0.1978	0.2894	0.1601
Fe	Fe13	0.9478118122552743	0.0390337101478027	0.2398286127199463
Fe	Fe14	0.4464423589457734	0.5403275822707859	0.2398294042229869
Fe	Fe15	0.9468415775570592	0.5394318086926254	0.2401281891591167
Fe	Fe16	0.4474020020856478	0.0399078449603555	0.2401223876732624
Fe	Fe17	0.1961812610085773	0.2896099216553202	0.3207019854422714
Fe	Fe18	0.6961762482369506	0.2896147887220881	0.3202008039233111
Fe	Fe19	0.1961493401590064	0.7896167959956242	0.3207725004212627
Fe	Fe20	0.6961353548000364	0.7896313386789967	0.3207015136097175
Fe	Fe21	0.4362669886559820	0.5489127587857033	0.4002742184580124
Fe	Fe22	0.9460854125271143	0.5401579235237699	0.4010926111155805
Fe	Fe23	0.4449392818937974	0.0389950511186589	0.4010994488601796
Fe	Fe24	0.9549534415035875	0.0301984602143734	0.4002673343610780

N	N25	0.7740578987109130	0.3679342744125110	0.4548709219953883
N	N26	0.6170773746760359	0.2111858801670572	0.4548460789012971

2.4 NH adsorption.cif

data_

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_cell_length_a 4.9052
_cell_length_b 4.9052
_cell_length_c 25.0126
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 70.5287

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

Fe	Fe1	0.1978	0.2894	0.0000
Fe	Fe2	0.6978	0.2894	0.0000
Fe	Fe3	0.1978	0.7894	0.0000
Fe	Fe4	0.6978	0.7894	0.0000
Fe	Fe5	0.4478	0.0394	0.0801
Fe	Fe6	0.4478	0.5394	0.0801
Fe	Fe7	0.9478	0.5394	0.0801
Fe	Fe8	0.9478	0.0394	0.0801
Fe	Fe9	0.1978	0.7894	0.1601
Fe	Fe10	0.6978	0.2894	0.1601

Fe	Fe11	0.6978	0.7894	0.1601
Fe	Fe12	0.1978	0.2894	0.1601
Fe	Fe13	0.9470193599932727	0.0396907357773327	0.2398611478597665
Fe	Fe14	0.4469633839665911	0.5397482892896899	0.2398610460725066
Fe	Fe15	0.9471314462999787	0.5398868292762713	0.2403507259580775
Fe	Fe16	0.4467533934937714	0.0395377640034041	0.2403513018953986
Fe	Fe17	0.1961560764655626	0.2899488784881349	0.3215118995526329
Fe	Fe18	0.6962027807540649	0.2898941186180597	0.3201761265404748
Fe	Fe19	0.1961820862568817	0.7899120456446106	0.3200363649476438
Fe	Fe20	0.6961590493137569	0.7899283186904287	0.3215077895539744
Fe	Fe21	0.4239270077662490	0.5619745431383709	0.4005431680816503
Fe	Fe22	0.9359527456047344	0.5302300378310003	0.4026058984338167
Fe	Fe23	0.4558699357406012	0.0498971939833648	0.4026179177143150
Fe	Fe24	0.9677860435048459	0.0182186141716675	0.4005275960490289
N	N25	0.6961575254911035	0.2904126300582131	0.4433675443188444
H	H26	0.6964072282033800	0.2904023119851812	0.4845037515157239

2.5 NH_2 adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 4.9052
_cell_length_b 4.9052
_cell_length_c 25.0126
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 70.5287

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.1978	0.2894	0.0000
Fe	Fe2	0.6978	0.2894	0.0000
Fe	Fe3	0.1978	0.7894	0.0000
Fe	Fe4	0.6978	0.7894	0.0000
Fe	Fe5	0.4478	0.0394	0.0801
Fe	Fe6	0.4478	0.5394	0.0801
Fe	Fe7	0.9478	0.5394	0.0801
Fe	Fe8	0.9478	0.0394	0.0801
Fe	Fe9	0.1978	0.7894	0.1601
Fe	Fe10	0.6978	0.2894	0.1601
Fe	Fe11	0.6978	0.7894	0.1601
Fe	Fe12	0.1978	0.2894	0.1601
Fe	Fe13	0.9485230541196070	0.0385854138607821	0.2401806671693231
Fe	Fe14	0.4466019042847315	0.5404009025679036	0.2401933541345477
Fe	Fe15	0.9472793330277470	0.5391880016297257	0.2398453531784740
Fe	Fe16	0.4479364004993517	0.0397953605635107	0.2398436447387879
Fe	Fe17	0.1971469407487367	0.2894048827200668	0.3199550504566923
Fe	Fe18	0.6971155848118098	0.2894186835883018	0.3211259850554195
Fe	Fe19	0.1970845881955806	0.7894777618618811	0.3216300199171068
Fe	Fe20	0.6970802233665359	0.7894663086104924	0.3199613239406386
Fe	Fe21	0.4450217195166574	0.5412306916782305	0.4038595762050681
Fe	Fe22	0.9537170599320287	0.5459206304939319	0.3981771209275486
Fe	Fe23	0.4401133604281586	0.0326986510271459	0.3982304070697207
Fe	Fe24	0.9486801427531368	0.0374732847896319	0.4039321742718778
N	N25	0.6957587080901436	0.2889464030372669	0.4608772766982181
H	H26	0.5930609765331368	0.1872042421928952	0.4858640420606648
H	H27	0.7975122229108004	0.3912576790387614	0.4859427288112370

2.6 NH_3 adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 4.9052
_cell_length_b 4.9052
_cell_length_c 25.0126
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 70.5287

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
Fe Fe1 0.1978 0.2894 0.0000
Fe Fe2 0.6978 0.2894 0.0000
Fe Fe3 0.1978 0.7894 0.0000
Fe Fe4 0.6978 0.7894 0.0000
Fe Fe5 0.4478 0.0394 0.0801
Fe Fe6 0.4478 0.5394 0.0801
Fe Fe7 0.9478 0.5394 0.0801
Fe Fe8 0.9478 0.0394 0.0801
Fe Fe9 0.1978 0.7894 0.1601
Fe Fe10 0.6978 0.2894 0.1601
Fe Fe11 0.6978 0.7894 0.1601
Fe Fe12 0.1978 0.2894 0.1601
Fe Fe13 0.9467854539149155 0.0394359732126888 0.2403774256252375
Fe Fe14 0.4469712805491178 0.5395756715031941 0.2400601621906655

Fe	Fe15	0.9469569592079189	0.5395280001452349	0.2399197804456157
Fe	Fe16	0.4469189119378592	0.0395339979682339	0.2399249693483190
Fe	Fe17	0.1965820463080446	0.2900382873798163	0.3202943194278313
Fe	Fe18	0.6931808970737655	0.2927037456567311	0.3209715824468490
Fe	Fe19	0.1991378391925580	0.7866908708992525	0.3209851063441986
Fe	Fe20	0.6956265862818759	0.7891995291287667	0.3203494962892473
Fe	Fe21	0.4457337466260821	0.5397659925061463	0.4070456396261729
Fe	Fe22	0.9459822456827789	0.5397685872478909	0.3994010287986085
Fe	Fe23	0.4455725693282633	0.0400511040189694	0.3994019315514968
Fe	Fe24	0.9454396797010582	0.0397963395753261	0.3988445095937769
N	N25	0.4414158895154249	0.5382014676185365	0.4928117884729966
H	H26	0.5247217474644308	0.3303142120531338	0.5068941675446973
H	H27	0.2339274607247638	0.6330140072015631	0.5064879387444168
H	H28	0.5674829948756061	0.6549365989730433	0.5059469809773048

2.7 N_2 activation.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 4.9052

_cell_length_b 4.9052

_cell_length_c 25.0126

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 70.5287

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.1978	0.2894	0.0000
Fe	Fe2	0.6978	0.2894	0.0000
Fe	Fe3	0.1978	0.7894	0.0000
Fe	Fe4	0.6978	0.7894	0.0000
Fe	Fe5	0.4478	0.0394	0.0801
Fe	Fe6	0.4478	0.5394	0.0801
Fe	Fe7	0.9478	0.5394	0.0801
Fe	Fe8	0.9478	0.0394	0.0801
Fe	Fe9	0.1978	0.7894	0.1601
Fe	Fe10	0.6978	0.2894	0.1601
Fe	Fe11	0.6978	0.7894	0.1601
Fe	Fe12	0.1978	0.2894	0.1601
Fe	Fe13	0.9470	0.0377	0.2404
Fe	Fe14	0.4453	0.5396	0.2406
Fe	Fe15	0.9464	0.5384	0.2402
Fe	Fe16	0.4464	0.0390	0.2400
Fe	Fe17	0.1961	0.2875	0.3198
Fe	Fe18	0.6958	0.2860	0.3219
Fe	Fe19	0.1905	0.7924	0.3222
Fe	Fe20	0.6943	0.7877	0.3203
Fe	Fe21	0.4439	0.5367	0.4026
Fe	Fe22	0.9761	0.5318	0.3987
Fe	Fe23	0.4282	0.0340	0.3991
Fe	Fe24	0.9210	0.0526	0.4088
N	N25	0.7550	0.4071	0.4486
N	N26	0.6913	0.7726	0.4423

2.8 N+H hydrogenation.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 4.9052

_cell_length_b 4.9052

_cell_length_c 25.0126

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 70.5287

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.1978	0.2894	0.0000
Fe	Fe2	0.6978	0.2894	0.0000
Fe	Fe3	0.1978	0.7894	0.0000
Fe	Fe4	0.6978	0.7894	0.0000
Fe	Fe5	0.4478	0.0394	0.0801
Fe	Fe6	0.4478	0.5394	0.0801
Fe	Fe7	0.9478	0.5394	0.0801
Fe	Fe8	0.9478	0.0394	0.0801
Fe	Fe9	0.1978	0.7894	0.1601
Fe	Fe10	0.6978	0.2894	0.1601
Fe	Fe11	0.6978	0.7894	0.1601
Fe	Fe12	0.1978	0.2894	0.1601
Fe	Fe13	0.9490918772898015	0.0359557089932745	0.2404708360293463
Fe	Fe14	0.4465340788940088	0.5384740212711938	0.2404850711820623
Fe	Fe15	0.9478357061529913	0.5371971539640714	0.2402756685485645
Fe	Fe16	0.4480720066057148	0.0373384044615166	0.2397945218479451
Fe	Fe17	0.1997334381869567	0.2826904210538279	0.3202712817573277

Fe Fe18 0.6988543883580771 0.2862684751486505 0.3210215749882139

Fe Fe19 0.1975630219910482 0.7849724981633563 0.3219003667825853

Fe Fe20 0.6952511108481930 0.7871100105822603 0.3202933453446067

Fe Fe21 0.4595371073843315 0.5196853167227383 0.4051617265936330

Fe Fe22 0.9601530321371043 0.5459993817211006 0.3959897232073031

Fe Fe23 0.4296638112897026 0.0155897632850506 0.3993959021754401

Fe Fe24 0.9341975803572116 0.0450518610170544 0.4051024990584134

N N25 0.5936807739624377 0.1787927876417213 0.4436441675420490

H H26 0.8494959391248621 0.4364211647976608 0.4478552521146570

2.9 HN+H hydrogenation.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 4.9052

_cell_length_b 4.9052

_cell_length_c 25.0126

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 70.5287

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe Fe1 0.1978 0.2894 0.0000

Fe Fe2 0.6978 0.2894 0.0000

Fe Fe3 0.1978 0.7894 0.0000

Fe	Fe4	0.6978	0.7894	0.0000
Fe	Fe5	0.4478	0.0394	0.0801
Fe	Fe6	0.4478	0.5394	0.0801
Fe	Fe7	0.9478	0.5394	0.0801
Fe	Fe8	0.9478	0.0394	0.0801
Fe	Fe9	0.1978	0.7894	0.1601
Fe	Fe10	0.6978	0.2894	0.1601
Fe	Fe11	0.6978	0.7894	0.1601
Fe	Fe12	0.1978	0.2894	0.1601
Fe	Fe13	0.9478421642504151	0.0397793686499268	0.2401635020184389
Fe	Fe14	0.4464770746572244	0.5408882750372428	0.2401566635641657
Fe	Fe15	0.9470007524434900	0.5400492521329778	0.2403655952159933
Fe	Fe16	0.4472305024487783	0.0405372648145099	0.2403129369459459
Fe	Fe17	0.1972289291730311	0.2910678556223238	0.3214965368864919
Fe	Fe18	0.6961378271331533	0.2910528534181522	0.3205025596822947
Fe	Fe19	0.1978038022393791	0.7908529541168337	0.3208992004416747
Fe	Fe20	0.6953405936339478	0.7918512593246763	0.3213369351183524
Fe	Fe21	0.4333201693206475	0.5581067108958102	0.4018269514639725
Fe	Fe22	0.9428776610677813	0.5409457574144527	0.4014556127227062
Fe	Fe23	0.4476587040630970	0.0485378041440662	0.4039941020620207
Fe	Fe24	0.9573357292191840	0.0220101301702458	0.4001728564514630
N	N25	0.6770507013107596	0.2760748877522718	0.4503689804528486
H	H26	0.6491636444156426	0.2783979467178955	0.4910441288931046
H	H27	0.9643669585018442	0.2440858021828068	0.4523101562844224

2.10 H_2N+H hydrogenation.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 4.9052

_cell_length_b 4.9052

_cell_length_c 25.0126

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 70.5287

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.1978	0.2894	0.0000
Fe	Fe2	0.6978	0.2894	0.0000
Fe	Fe3	0.1978	0.7894	0.0000
Fe	Fe4	0.6978	0.7894	0.0000
Fe	Fe5	0.4478	0.0394	0.0801
Fe	Fe6	0.4478	0.5394	0.0801
Fe	Fe7	0.9478	0.5394	0.0801
Fe	Fe8	0.9478	0.0394	0.0801
Fe	Fe9	0.1978	0.7894	0.1601
Fe	Fe10	0.6978	0.2894	0.1601
Fe	Fe11	0.6978	0.7894	0.1601
Fe	Fe12	0.1978	0.2894	0.1601
Fe	Fe13	0.9476544862031389	0.0390338600342865	0.2401410806241319
Fe	Fe14	0.4475239823912716	0.5388013674634109	0.2400253370696137
Fe	Fe15	0.9473219928788938	0.5391334632569998	0.2397976581737438
Fe	Fe16	0.4474013517274299	0.0386266484159371	0.2399886738237013
Fe	Fe17	0.1961027275054522	0.2914640355618929	0.3201426873012458
Fe	Fe18	0.6973354023309298	0.2890579905466446	0.3209601285850782
Fe	Fe19	0.2002073222303329	0.7846211623500315	0.3212361570902899
Fe	Fe20	0.6980045392663787	0.7874179237417551	0.3203338321203198
Fe	Fe21	0.4513936341353024	0.5363306810004080	0.4053451371698228

Fe Fe22 0.9516361190184095 0.5328989840527945 0.4007391549274957

Fe Fe23 0.4415079052884196 0.0501226996632430 0.3976893630041974

Fe Fe24 0.9514719150451546 0.0269154345718274 0.3999472817155634

N N25 0.6870632826689166 0.5949760150319492 0.4713995132434236

H H26 0.8749269380860506 0.7364352611609790 0.4570199353785984

H H27 0.7722625200754794 0.4227218185698290 0.4967872613153421

H H28 0.5638649127761020 0.7694071221074109 0.4934329072181035

3. (111) surface

3.1 H adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 8.0101

_cell_length_b 8.0101

_cell_length_c 23.9928

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 120.0000

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe Fe1 0.3333299999999966 0.1666700000000034 0.0340699999999998

Fe Fe2 0.1666700000000034 0.3333299999999966 0.1022200000000026

Fe Fe3 0.0000000000000000 0.0000000000000000 0.1703699999999984

Fe	Fe4	0.3330986210705048	0.1665496849791761	0.2384532435627904
Fe	Fe5	0.1665972979348443	0.3347769061942776	0.3109992881426166
Fe	Fe6	0.0035836882680805	0.0017905056693352	0.3716847953649168
Fe	Fe7	0.1666700000000034	0.3333299999999966	0.0000000000000000
Fe	Fe8	0.0000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe9	0.3333299999999966	0.1666700000000034	0.1362999999999985
Fe	Fe10	0.1667574145434740	0.3336090653212807	0.2049831058725377
Fe	Fe11	0.0013071436690481	0.0006532470631388	0.2734351943839539
Fe	Fe12	0.3332166699970550	0.1666076502772105	0.3378774218128232
Fe	Fe13	0.8333299999999966	0.1666700000000034	0.0340699999999998
Fe	Fe14	0.6666700000000034	0.3333299999999966	0.1022200000000026
Fe	Fe15	0.5000000000000000	0.0000000000000000	0.1703699999999984
Fe	Fe16	0.8333794285397094	0.1662592437836413	0.2393583238276345
Fe	Fe17	0.6697279753054587	0.3348640593358824	0.3100055182386824
Fe	Fe18	0.4962211768214163	0.0085974949227456	0.3728159973594433
Fe	Fe19	0.6666700000000034	0.3333299999999966	0.0000000000000000
Fe	Fe20	0.5000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe21	0.8333299999999966	0.1666700000000034	0.1362999999999985
Fe	Fe22	0.6669057373287621	0.3334534818925843	0.2048706724128771
Fe	Fe23	0.4998276820975781	0.0002467077650328	0.2736352860774264
Fe	Fe24	0.8329551574119899	0.1666608651124024	0.3396603268023053
Fe	Fe25	0.3333299999999966	0.6666700000000034	0.0340699999999998
Fe	Fe26	0.1666700000000034	0.8333299999999966	0.1022200000000026
Fe	Fe27	0.0000000000000000	0.5000000000000000	0.1703699999999984
Fe	Fe28	0.3343010582647299	0.6671501003184774	0.2396428220618254
Fe	Fe29	0.1665974485156080	0.8318198917797696	0.3109991324266022
Fe	Fe30	0.0021908793071852	0.5010947551172882	0.3722866067813787
Fe	Fe31	0.1666700000000034	0.8333299999999966	0.0000000000000000
Fe	Fe32	0.0000000000000000	0.5000000000000000	0.0681500000000028
Fe	Fe33	0.3333299999999966	0.6666700000000034	0.1362999999999985
Fe	Fe34	0.1667571577364952	0.8331483652943923	0.2049828309490221
Fe	Fe35	0.0009248401482381	0.5004621373109319	0.2731520719470131
Fe	Fe36	0.3373986005828427	0.6686984409899578	0.3405584375615913

Fe	Fe37	0.8333299999999966	0.6666700000000034	0.0340699999999998
Fe	Fe38	0.6666700000000034	0.8333299999999966	0.1022200000000026
Fe	Fe39	0.5000000000000000	0.5000000000000000	0.1703699999999984
Fe	Fe40	0.8333789773687280	0.6671198570797654	0.2393581517510892
Fe	Fe41	0.6671326867460592	0.8335657408767081	0.3117988966406545
Fe	Fe42	0.4962167240698475	0.4876179607624698	0.3728171553574076
Fe	Fe43	0.6666700000000034	0.8333299999999966	0.0000000000000000
Fe	Fe44	0.5000000000000000	0.5000000000000000	0.0681500000000028
Fe	Fe45	0.8333299999999966	0.6666700000000034	0.1362999999999985
Fe	Fe46	0.6668101790870912	0.8334048656035862	0.2052059451538388
Fe	Fe47	0.4998274589945674	0.4995805033695471	0.2736357875602881
Fe	Fe48	0.8329540565000833	0.6662926298905714	0.3396601723064275
H	H49	0.4187954085898783	0.2093982482550451	0.4005713960397143

3.2 N adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 8.0101
_cell_length_b 8.0101
_cell_length_c 23.9928
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 120.0000

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.3333	0.1667	0.0341
Fe	Fe2	0.1667	0.3333	0.1022
Fe	Fe3	0.0000	0.0000	0.1704
Fe	Fe4	0.3340	0.1660	0.2390
Fe	Fe5	0.1668	0.3332	0.3138
Fe	Fe6	0.0106	0.0152	0.3739
Fe	Fe7	0.1667	0.3333	0.0000
Fe	Fe8	0.0000	0.0000	0.0681
Fe	Fe9	0.3333	0.1667	0.1363
Fe	Fe10	0.1672	0.3328	0.2058
Fe	Fe11	0.0000	-0.0002	0.2738
Fe	Fe12	0.3457	0.1542	0.3366
Fe	Fe13	0.8333	0.1667	0.0341
Fe	Fe14	0.6667	0.3333	0.1022
Fe	Fe15	0.5000	0.0000	0.1704
Fe	Fe16	0.8338	0.1664	0.2392
Fe	Fe17	0.6701	0.3375	0.3102
Fe	Fe18	0.5031	0.9968	0.3710
Fe	Fe19	0.6667	0.3333	0.0000
Fe	Fe20	0.5000	0.0000	0.0681
Fe	Fe21	0.8333	0.1667	0.1363
Fe	Fe22	0.6667	0.3336	0.2050
Fe	Fe23	0.5015	0.9985	0.2721
Fe	Fe24	0.8310	0.1668	0.3388
Fe	Fe25	0.3333	0.6667	0.0341
Fe	Fe26	0.1667	0.8333	0.1022
Fe	Fe27	0.0000	0.5000	0.1704
Fe	Fe28	0.3336	0.6661	0.2392
Fe	Fe29	0.1625	0.8299	0.3102
Fe	Fe30	0.9955	0.5045	0.3708
Fe	Fe31	0.1667	0.8333	0.0000

Fe	Fe32	0.0000	0.5000	0.0681
Fe	Fe33	0.3333	0.6667	0.1363
Fe	Fe34	0.1664	0.8333	0.2050
Fe	Fe35	-0.0001	0.5000	0.2730
Fe	Fe36	0.3332	0.6689	0.3388
Fe	Fe37	0.8333	0.6667	0.0341
Fe	Fe38	0.6667	0.8333	0.1022
Fe	Fe39	0.5000	0.5000	0.1704
Fe	Fe40	0.8329	0.6671	0.2396
Fe	Fe41	0.6668	0.8331	0.3114
Fe	Fe42	0.4847	0.4893	0.3739
Fe	Fe43	0.6667	0.8333	0.0000
Fe	Fe44	0.5000	0.5000	0.0681
Fe	Fe45	0.8333	0.6667	0.1363
Fe	Fe46	0.6669	0.8331	0.2050
Fe	Fe47	0.5001	0.5000	0.2738
Fe	Fe48	0.8296	0.6704	0.3408
N	N49	0.2437	0.2562	0.3809

3.3 N_2 adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 8.0101

_cell_length_b 8.0101

_cell_length_c 23.9928

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 120.0000

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.3333299999999966	0.1666700000000034	0.0340699999999998
Fe	Fe2	0.1666700000000034	0.3333299999999966	0.1022200000000026
Fe	Fe3	0.0000000000000000	0.0000000000000000	0.1703699999999984
Fe	Fe4	0.3322801992458684	0.1656009648489212	0.2404209613344689
Fe	Fe5	0.1638523593721735	0.3313522122815980	0.3103972194053939
Fe	Fe6	0.9884726547271737	0.9932390483573960	0.3710672373274789
Fe	Fe7	0.1666700000000034	0.3333299999999966	0.0000000000000000
Fe	Fe8	0.0000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe9	0.3333299999999966	0.1666700000000034	0.1362999999999985
Fe	Fe10	0.1662277312032662	0.3318594480665130	0.2049854481723631
Fe	Fe11	-0.0002022057674246	0.9991535716635523	0.2734431531699645
Fe	Fe12	0.3338063557083868	0.1656573062598529	0.3431321435973019
Fe	Fe13	0.8333299999999966	0.1666700000000034	0.0340699999999998
Fe	Fe14	0.6666700000000034	0.3333299999999966	0.1022200000000026
Fe	Fe15	0.5000000000000000	0.0000000000000000	0.1703699999999984
Fe	Fe16	0.8309565688721201	0.1642138856423473	0.2388514182070759
Fe	Fe17	0.6666692995357671	0.3324390825056137	0.3076335976334081
Fe	Fe18	0.5042583281293804	0.9845209943235618	0.3761897415354181
Fe	Fe19	0.6666700000000034	0.3333299999999966	0.0000000000000000
Fe	Fe20	0.5000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe21	0.8333299999999966	0.1666700000000034	0.1362999999999985
Fe	Fe22	0.6651715459533057	0.3323095636342321	0.2047491668666220
Fe	Fe23	0.4969114860819836	0.9976779167430185	0.2745081600180900
Fe	Fe24	0.8299669870213716	0.1663642979963816	0.3385695885624112
Fe	Fe25	0.3333299999999966	0.6666700000000034	0.0340699999999998
Fe	Fe26	0.1666700000000034	0.8333299999999966	0.1022200000000026
Fe	Fe27	0.0000000000000000	0.5000000000000000	0.1703699999999984

Fe	Fe28	0.3335792938080165	0.6662807405669244	0.2389506247510929
Fe	Fe29	0.1637118909421865	0.8304089685602221	0.3104143342257473
Fe	Fe30	0.0001524998984368	0.4988636440595006	0.3719226846422851
Fe	Fe31	0.1666700000000034	0.8333299999999966	0.0000000000000000
Fe	Fe32	0.0000000000000000	0.5000000000000000	0.0681500000000028
Fe	Fe33	0.3333299999999966	0.6666700000000034	0.1362999999999985
Fe	Fe34	0.1662435550148739	0.8337935877772572	0.2050038239589106
Fe	Fe35	0.9994399752598504	0.4990047581670232	0.2725888707714417
Fe	Fe36	0.3305492948138123	0.6640576810710501	0.3381332090353228
Fe	Fe37	0.8333299999999966	0.6666700000000034	0.0340699999999998
Fe	Fe38	0.6666700000000034	0.8333299999999966	0.1022200000000026
Fe	Fe39	0.5000000000000000	0.5000000000000000	0.1703699999999984
Fe	Fe40	0.8309588925833895	0.6657395351685855	0.2388670218765498
Fe	Fe41	0.6643692149427202	0.8311881261358683	0.3115019644155667
Fe	Fe42	0.5037092880035718	0.5162501992097132	0.3762126122239505
Fe	Fe43	0.6666700000000034	0.8333299999999966	0.0000000000000000
Fe	Fe44	0.5000000000000000	0.5000000000000000	0.0681500000000028
Fe	Fe45	0.8333299999999966	0.6666700000000034	0.1362999999999985
Fe	Fe46	0.6661738670750638	0.8327775930294381	0.2051737876118441
Fe	Fe47	0.4969343514687704	0.4976769215974389	0.2744754264345066
Fe	Fe48	0.8298346966531068	0.6615104352224840	0.3386415468260465
N	N49	0.4643036074636105	0.3059989941820524	0.4191240118882257
N	N50	0.4643331859478271	0.1546626179486728	0.4190950113369187

3.4 NH adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 8.0101

_cell_length_b 8.0101

_cell_length_c 23.9928

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 120.0000

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe3	0.0000000000000000	0.0000000000000000	0.1703699999999984
Fe	Fe4	0.3341163869361491	0.1658839514128255	0.2394681685474605
Fe	Fe5	0.1666697778715690	0.3333300345415666	0.3145502031462442
Fe	Fe6	0.0006259522087376	0.0011292094034757	0.3719540001405927
Fe	Fe7	0.1666700000000034	0.3333299999999966	0.0000000000000000
Fe	Fe8	0.0000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe9	0.3333299999999966	0.1666700000000034	0.1362999999999985
Fe	Fe10	0.1667276807773512	0.3332724287427809	0.2063917962473375
Fe	Fe11	0.0009604617156930	0.0007621040960431	0.2733142342604858
Fe	Fe12	0.3438513359041381	0.1561469763607132	0.3394449386700887
Fe	Fe13	0.8333299999999966	0.1666700000000034	0.0340699999999998
Fe	Fe14	0.6666700000000034	0.3333299999999966	0.1022200000000026
Fe	Fe15	0.5000000000000000	0.0000000000000000	0.1703699999999984
Fe	Fe16	0.8332143772625360	0.1665994562218598	0.2393124992253340
Fe	Fe17	0.6680630037992062	0.3351095740062694	0.3099872495817644
Fe	Fe18	0.5042958512627338	0.9957042230120542	0.3718760886084423
Fe	Fe19	0.6666700000000034	0.3333299999999966	0.0000000000000000
Fe	Fe20	0.5000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe21	0.8333299999999966	0.1666700000000034	0.1362999999999985
Fe	Fe22	0.6665101731944542	0.3332338035180155	0.2048717682498582

Fe	Fe23	0.5008736368881593	0.9991264476268182	0.2726850477900641
Fe	Fe24	0.8314641400696715	0.1682196990872921	0.3391778674436807
Fe	Fe25	0.3333299999999966	0.6666700000000034	0.0340699999999998
Fe	Fe26	0.1666700000000034	0.8333299999999966	0.1022200000000026
Fe	Fe27	0.0000000000000000	0.5000000000000000	0.1703699999999984
Fe	Fe28	0.3334006411739966	0.6667855814684279	0.2393126863021770
Fe	Fe29	0.1648910366591254	0.8319361493967820	0.3099872258953106
Fe	Fe30	0.9931182827792475	0.5068818055047370	0.3706851638532008
Fe	Fe31	0.1666700000000034	0.8333299999999966	0.0000000000000000
Fe	Fe32	0.0000000000000000	0.5000000000000000	0.0681500000000028
Fe	Fe33	0.3333299999999966	0.6666700000000034	0.1362999999999985
Fe	Fe34	0.1667669757080841	0.8334902583191423	0.2048718119726494
Fe	Fe35	0.0002890885158550	0.4997127142261092	0.2729624002949103
Fe	Fe36	0.3317816006791267	0.6685362077438862	0.3391778213903913
Fe	Fe37	0.8333299999999966	0.6666700000000034	0.0340699999999998
Fe	Fe38	0.6666700000000034	0.8333299999999966	0.1022200000000026
Fe	Fe39	0.5000000000000000	0.5000000000000000	0.1703699999999984
Fe	Fe40	0.8327880823687335	0.6672121674516878	0.2389294928327844
Fe	Fe41	0.6660073053409012	0.8339925516635204	0.3113373967121839
Fe	Fe42	0.4988708316356792	0.4993721416152133	0.3719537920031500
Fe	Fe43	0.6666700000000034	0.8333299999999966	0.0000000000000000
Fe	Fe44	0.5000000000000000	0.5000000000000000	0.0681500000000028
Fe	Fe45	0.8333299999999966	0.6666700000000034	0.1362999999999985
Fe	Fe46	0.6665221518996515	0.8334777450329993	0.2048966414371809
Fe	Fe47	0.4992383642486621	0.4990399565863208	0.2733144048252727
Fe	Fe48	0.8302804231662700	0.6697190150878067	0.3385888205278380
N	N49	0.2381862088049760	0.2618128054391352	0.3877168188266198
H	H50	0.2176102883951414	0.2823909712863700	0.4289967049259671

3.5 NH_2 adsorption.cif

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_cell_length_a 8.0101

_cell_length_b 8.0101

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_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

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loop_

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_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.1666700000000034	0.3333299999999966	0.1022200000000026
Fe	Fe3	0.0000000000000000	0.0000000000000000	0.1703699999999984
Fe	Fe4	0.3332747424169761	0.1666747208766168	0.2406535355628471
Fe	Fe5	0.1661833733872687	0.3332056448060518	0.3095030070821485
Fe	Fe6	0.9922513327216064	0.9942955824980287	0.3710985381493162
Fe	Fe7	0.1666700000000034	0.3333299999999966	0.0000000000000000
Fe	Fe8	0.0000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe9	0.3333299999999966	0.1666700000000034	0.1362999999999985
Fe	Fe10	0.1669171598403364	0.3326870901229450	0.2048845417108479
Fe	Fe11	0.0014588529838451	0.0002519643621899	0.2732742470328152
Fe	Fe12	0.3339256317295119	0.1692633274664256	0.3438725454697766
Fe	Fe13	0.8333299999999966	0.1666700000000034	0.0340699999999998
Fe	Fe14	0.6666700000000034	0.3333299999999966	0.1022200000000026
Fe	Fe15	0.5000000000000000	0.0000000000000000	0.1703699999999984
Fe	Fe16	0.8329748983947627	0.1662081440217467	0.2388086238016073
Fe	Fe17	0.6661038518362059	0.3329973324084050	0.3098493256665701

Fe	Fe18	0.5024262978835935	0.9947236966026726	0.3709858331940409
Fe	Fe19	0.6666700000000034	0.3333299999999966	0.0000000000000000
Fe	Fe20	0.5000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe21	0.8333299999999966	0.1666700000000034	0.1362999999999985
Fe	Fe22	0.6656131531603772	0.3326528896861484	0.2049298090434885
Fe	Fe23	0.4985600391999664	0.0003078887250922	0.2732754402082457
Fe	Fe24	0.8340649932774922	0.1680524532188695	0.3381621278348956
Fe	Fe25	0.3333299999999966	0.6666700000000034	0.0340699999999998
Fe	Fe26	0.1666700000000034	0.8333299999999966	0.1022200000000026
Fe	Fe27	0.0000000000000000	0.5000000000000000	0.1703699999999984
Fe	Fe28	0.3338945898961663	0.6669146658938374	0.2389625751697925
Fe	Fe29	0.1680135043147555	0.8361812885778458	0.3109918456756123
Fe	Fe30	0.9998085541243777	0.5003931626249246	0.3716711561991279
Fe	Fe31	0.1666700000000034	0.8333299999999966	0.0000000000000000
Fe	Fe32	0.0000000000000000	0.5000000000000000	0.0681500000000028
Fe	Fe33	0.3333299999999966	0.6666700000000034	0.1362999999999985
Fe	Fe34	0.1671503620694904	0.8343349675328114	0.2050185226889728
Fe	Fe35	0.0003783282734237	0.5012624040828367	0.2728448763538660
Fe	Fe36	0.3334426762882944	0.6650387768226211	0.3384833615631307
Fe	Fe37	0.8333299999999966	0.6666700000000034	0.0340699999999998
Fe	Fe38	0.6666700000000034	0.8333299999999966	0.1022200000000026
Fe	Fe39	0.5000000000000000	0.5000000000000000	0.1703699999999984
Fe	Fe40	0.8328384054239858	0.6669274161411683	0.2389686446691768
Fe	Fe41	0.6666953264150830	0.8337422220416926	0.3104662889046903
Fe	Fe42	0.5026422904776182	0.5053026748072877	0.3723266096464178
Fe	Fe43	0.6666700000000034	0.8333299999999966	0.0000000000000000
Fe	Fe44	0.5000000000000000	0.5000000000000000	0.0681500000000028
Fe	Fe45	0.8333299999999966	0.6666700000000034	0.1362999999999985
Fe	Fe46	0.6665308504324521	0.8331939842567239	0.2049353273310505
Fe	Fe47	0.4995738097133876	0.4992394840995717	0.2733426115974882
Fe	Fe48	0.8312781333988269	0.6653736145071665	0.3384586752271987
N	N49	0.3816712428023648	0.2803748605550592	0.4212886206336617
H	H50	0.4700213906697193	0.2572783845724539	0.4471477332759633

H H51 0.2668921512887377 0.2654473355529727 0.4442219238275797

3.6 NH_3 adsorption.cif

data_

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_cell_length_c 23.9928
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_cell_angle_beta 90.0000
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_symmetry_space_group_name_H-M 'T'

loop_
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_atom_site_label
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Fe Fe2 0.1666700000000034 0.3333299999999966 0.1022200000000026
Fe Fe3 0.0000000000000000 0.0000000000000000 0.1703699999999984
Fe Fe4 0.3336725898993617 0.1673722039257132 0.2391949132490460
Fe Fe5 0.1669768681768524 0.3335052463137241 0.3107880087768995
Fe Fe6 0.0004523245999234 0.9995642635821272 0.3715241928394976
Fe Fe7 0.1666700000000034 0.3333299999999966 0.0000000000000000
Fe Fe8 0.0000000000000000 0.0000000000000000 0.0681500000000028
Fe Fe9 0.3333299999999966 0.1666700000000034 0.1362999999999985
Fe Fe10 0.1663102359645894 0.3331572796656266 0.2049800556989740
Fe Fe11 0.0000736129513898 -0.0000740322165415 0.2733056918033496

Fe	Fe12	0.3337711618894033	0.1675988481766091	0.3391115598509384
Fe	Fe13	0.8333299999999966	0.1666700000000034	0.0340699999999998
Fe	Fe14	0.6666700000000034	0.3333299999999966	0.1022200000000026
Fe	Fe15	0.5000000000000000	0.0000000000000000	0.1703699999999984
Fe	Fe16	0.8333084542709377	0.1666758802714533	0.2391718825088009
Fe	Fe17	0.6664911912571362	0.3335123748575453	0.3107919278138843
Fe	Fe18	0.4990576138338844	0.9995684757758798	0.3715096722547591
Fe	Fe19	0.6666700000000034	0.3333299999999966	0.0000000000000000
Fe	Fe20	0.5000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe21	0.8333299999999966	0.1666700000000034	0.1362999999999985
Fe	Fe22	0.6668333643487446	0.3331651777062797	0.2049821060386010
Fe	Fe23	0.4998031898670154	0.9999097782804350	0.2733017614800489
Fe	Fe24	0.8333178348245653	0.1666822895172393	0.3393596845753238
Fe	Fe25	0.3333299999999966	0.6666700000000034	0.0340699999999998
Fe	Fe26	0.1666700000000034	0.8333299999999966	0.1022200000000026
Fe	Fe27	0.0000000000000000	0.5000000000000000	0.1703699999999984
Fe	Fe28	0.3336866031980390	0.6663053882800990	0.2391971530062090
Fe	Fe29	0.1666603943439749	0.8333511277541504	0.3112264661717478
Fe	Fe30	0.0004233058826839	0.5009488174167072	0.3715148967376473
Fe	Fe31	0.1666700000000034	0.8333299999999966	0.0000000000000000
Fe	Fe32	0.0000000000000000	0.5000000000000000	0.0681500000000028
Fe	Fe33	0.3333299999999966	0.6666700000000034	0.1362999999999985
Fe	Fe34	0.1666758115568790	0.8333353808451460	0.2052317564033579
Fe	Fe35	0.0000879172437435	0.5001929402139533	0.2733026978438187
Fe	Fe36	0.3337816076681785	0.6662029943815440	0.3391170569611536
Fe	Fe37	0.8333299999999966	0.6666700000000034	0.0340699999999998
Fe	Fe38	0.6666700000000034	0.8333299999999966	0.1022200000000026
Fe	Fe39	0.5000000000000000	0.5000000000000000	0.1703699999999984
Fe	Fe40	0.8326354953648879	0.6663294379872220	0.2391931565470103
Fe	Fe41	0.6664941297004696	0.8330184869472294	0.3107892352876247
Fe	Fe42	0.5000149548550220	0.5000254616698097	0.3732987783959078
Fe	Fe43	0.6666700000000034	0.8333299999999966	0.0000000000000000
Fe	Fe44	0.5000000000000000	0.5000000000000000	0.0681500000000028

Fe	Fe45	0.8333299999999966	0.6666700000000034	0.1362999999999985
Fe	Fe46	0.6668393763688615	0.8336847050839206	0.2049803534636289
Fe	Fe47	0.4999995505054283	0.4999992018846919	0.2733617538789618
Fe	Fe48	0.8324190622119922	0.6662410329971301	0.3391079157108012
N	N49	0.4998773429974978	0.5007026798339178	0.4602523227255719
H	H50	0.4287130267082063	0.5686390938543365	0.4746354512165407
H	H51	0.4320679390207074	0.3619020186553223	0.4748714435277009
H	H52	0.6388008300951151	0.5720034386421970	0.4747542217759387

3.7 N_2 activation.cif

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_cell_length_c          23.9928
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loop_
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Fe      Fe2          0.1667      0.3333      0.1022
Fe      Fe3          0.0000      0.0000      0.1704
Fe      Fe4          0.3307      0.1651      0.2388
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Fe	Fe5	0.1659	0.3355	0.3113
Fe	Fe6	0.0029	0.0010	0.3721
Fe	Fe7	0.1667	0.3333	0.0000
Fe	Fe8	0.0000	0.0000	0.0681
Fe	Fe9	0.3333	0.1667	0.1363
Fe	Fe10	0.1655	0.3331	0.2051
Fe	Fe11	0.9984	0.9990	0.2730
Fe	Fe12	0.3253	0.1623	0.3378
Fe	Fe13	0.8333	0.1667	0.0341
Fe	Fe14	0.6667	0.3333	0.1022
Fe	Fe15	0.5000	-0.0000	0.1704
Fe	Fe16	0.8327	0.1652	0.2394
Fe	Fe17	0.6610	0.3302	0.3087
Fe	Fe18	0.4948	0.0055	0.3730
Fe	Fe19	0.6667	0.3333	0.0000
Fe	Fe20	0.5000	-0.0000	0.0681
Fe	Fe21	0.8333	0.1667	0.1363
Fe	Fe22	0.6654	0.3326	0.2059
Fe	Fe23	0.4983	0.9980	0.2733
Fe	Fe24	0.8369	0.1612	0.3392
Fe	Fe25	0.3333	0.6667	0.0341
Fe	Fe26	0.1667	0.8333	0.1022
Fe	Fe27	0.0000	0.5000	0.1704
Fe	Fe28	0.3313	0.6655	0.2398
Fe	Fe29	0.1659	0.8298	0.3113
Fe	Fe30	0.9999	0.4996	0.3750
Fe	Fe31	0.1667	0.8333	0.0000
Fe	Fe32	0.0000	0.5000	0.0681
Fe	Fe33	0.3333	0.6667	0.1363
Fe	Fe34	0.1655	0.8322	0.2051
Fe	Fe35	0.9989	0.4992	0.2740
Fe	Fe36	0.3309	0.6651	0.3409
Fe	Fe37	0.8333	0.6667	0.0341

Fe	Fe38	0.6667	0.8333	0.1022
Fe	Fe39	0.5000	0.5000	0.1704
Fe	Fe40	0.8327	0.6671	0.2394
Fe	Fe41	0.6631	0.8312	0.3106
Fe	Fe42	0.4948	0.4885	0.3731
Fe	Fe43	0.6667	0.8333	0.0000
Fe	Fe44	0.5000	0.5000	0.0681
Fe	Fe45	0.8333	0.6667	0.1363
Fe	Fe46	0.6658	0.8328	0.2052
Fe	Fe47	0.4983	0.4997	0.2733
Fe	Fe48	0.8368	0.6748	0.3392
N	N49	0.7158	0.2525	0.3848
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3.8 N+H hydrogenation.cif

data_

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_cell_length_c 23.9928

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 120.0000

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loop_

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_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe3	0.0000000000000000	0.0000000000000000	0.1703699999999984
Fe	Fe4	0.3341824557305232	0.1667401747731571	0.2392412933937162
Fe	Fe5	0.1658118059545564	0.3328971138631009	0.3107298080395131
Fe	Fe6	1.0082228915947227	0.0143176156361545	0.3742702293225523
Fe	Fe7	0.1666700000000037	0.3333299999999989	0.0000000000000000
Fe	Fe8	0.0000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe9	0.3333299999999971	0.1666700000000036	0.1362999999999997
Fe	Fe10	0.1668518553203718	0.3337189251154365	0.2056885609837706
Fe	Fe11	0.0006818652989160	1.0006939799123538	0.2737694801888007
Fe	Fe12	0.3446310205833612	0.1601608887920802	0.3380895478309899
Fe	Fe13	0.8333300000000023	0.1666700000000058	0.0340699999999998
Fe	Fe14	0.6666700000000044	0.3333299999999970	0.1022200000000026
Fe	Fe15	0.5000000000000036	-0.0000000000000004	0.1703699999999984
Fe	Fe16	0.8330507769868242	0.1670786412168012	0.2392224271272182
Fe	Fe17	0.6698538506964677	0.3391079075521284	0.3107514368386287
Fe	Fe18	0.5019577373086846	-0.0041622711059547	0.3710014582433066
Fe	Fe19	0.6666700000000044	0.3333299999999970	0.0000000000000000
Fe	Fe20	0.5000000000000036	-0.0000000000000004	0.0681500000000028
Fe	Fe21	0.8333300000000023	0.1666700000000058	0.1362999999999997
Fe	Fe22	0.6663856750714398	0.3337829158116816	0.2049598287350860
Fe	Fe23	0.5008410186429757	0.9998779320859584	0.2726342613997772
Fe	Fe24	0.8322609593560687	0.1695792186725155	0.3387301203381066
Fe	Fe25	0.3333299999999971	0.6666700000000043	0.0340699999999998
Fe	Fe26	0.1666700000000037	0.8333299999999967	0.1022200000000026
Fe	Fe27	0.0000000000000000	0.5000000000000047	0.1703699999999984
Fe	Fe28	0.3338620466066178	0.6675817623818834	0.2393416017917911
Fe	Fe29	0.1648331319713051	0.8325694239004024	0.3104512731604123
Fe	Fe30	0.9963340590755088	0.5066010784349908	0.3714452096345396
Fe	Fe31	0.1666700000000037	0.8333299999999967	0.0000000000000000
Fe	Fe32	0.0000000000000000	0.5000000000000047	0.0681500000000028

Fe	Fe33	0.3333299999999971	0.6666700000000043	0.1362999999999997
Fe	Fe34	0.1666592486303755	0.8340553242026482	0.2050156466998564
Fe	Fe35	0.0000067405075707	0.5015663666312224	0.2727939087353327
Fe	Fe36	0.3305964780343232	0.6654071492161449	0.3396036404176391
Fe	Fe37	0.8333300000000023	0.6666700000000088	0.0340699999999998
Fe	Fe38	0.6666700000000044	0.8333299999999968	0.1022200000000026
Fe	Fe39	0.5000000000000036	0.5000000000000033	0.1703699999999984
Fe	Fe40	0.8330254342266146	0.6681719110771951	0.2395154319116847
Fe	Fe41	0.6664646523986475	0.8347138349503216	0.3117080957079150
Fe	Fe42	0.4990341528320981	0.4976022017136638	0.3740389799316637
Fe	Fe43	0.6666700000000044	0.8333299999999968	0.0000000000000000
Fe	Fe44	0.5000000000000036	0.5000000000000033	0.0681500000000028
Fe	Fe45	0.8333300000000023	0.6666700000000088	0.1362999999999997
Fe	Fe46	0.6667093986179723	0.8338167882420446	0.2050472712884239
Fe	Fe47	0.5008109804649612	0.5010317577960466	0.2735256564222709
Fe	Fe48	0.8318649723207332	0.6734586553637895	0.3401855240781816
N	N49	0.2410614503459108	0.2594566655570467	0.3855930288654308
H	H50	0.2281032345938305	0.4161439702577160	0.3854117505202907

3.9 HN+H hydrogenation.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 8.0101

_cell_length_b 8.0101

_cell_length_c 23.9928

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 120.0000

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.3333299999999971	0.1666700000000036	0.0340699999999998
Fe	Fe2	0.1666700000000037	0.3333300000000039	0.1022200000000026
Fe	Fe3	0.0000000000000000	0.0000000000000000	0.1703699999999984
Fe	Fe4	0.3354625814911109	0.1661503112093594	0.2395332749938503
Fe	Fe5	0.1679514925199727	0.3373821010754235	0.3064627360257066
Fe	Fe6	0.0078632687135890	0.0049204806539834	0.3735767466434339
Fe	Fe7	0.1666700000000037	0.3333300000000039	0.0000000000000000
Fe	Fe8	0.0000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe9	0.3333299999999971	0.1666700000000036	0.1363000000000008
Fe	Fe10	0.1674250762696893	0.3332555331079692	0.2045634243313044
Fe	Fe11	0.0019110433366016	-0.0005212750556707	0.2735678431526871
Fe	Fe12	0.3387846637653630	0.1616143109384933	0.3400566989351752
Fe	Fe13	0.8333300000000222	0.1666700000000161	0.0340699999999998
Fe	Fe14	0.6666700000000044	0.3333299999999970	0.1022200000000026
Fe	Fe15	0.5000000000000036	-0.0000000000000004	0.1703699999999984
Fe	Fe16	0.8340646654130340	0.1660983254472705	0.2394428068129331
Fe	Fe17	0.6701131060725525	0.3347683798010382	0.3112852836407869
Fe	Fe18	0.5080170570982453	-0.0005630238767438	0.3713191559754792
Fe	Fe19	0.6666700000000044	0.3333299999999970	0.0000000000000000
Fe	Fe20	0.5000000000000036	-0.0000000000000004	0.0681500000000028
Fe	Fe21	0.8333300000000222	0.1666700000000161	0.1363000000000008
Fe	Fe22	0.6672095589504791	0.3334774799191109	0.2051140380775719
Fe	Fe23	0.5025333256065554	0.0005735977502105	0.2733349579023288
Fe	Fe24	0.8432968285475584	0.1716270873441886	0.3403722995398469
Fe	Fe25	0.3333299999999971	0.6666700000000043	0.0340699999999998
Fe	Fe26	0.1666700000000037	0.8333299999999967	0.1022200000000026
Fe	Fe27	0.0000000000000000	0.5000000000000071	0.1703699999999984

Fe	Fe28	0.3354198919146740	0.6678443577888160	0.2389042692443920
Fe	Fe29	0.1643124475492618	0.8317382462310434	0.3111835188090741
Fe	Fe30	0.0048559202731754	0.5026584638146998	0.3727276613223807
Fe	Fe31	0.1666700000000037	0.8333299999999967	0.0000000000000000
Fe	Fe32	0.0000000000000000	0.5000000000000071	0.0681500000000028
Fe	Fe33	0.3333299999999971	0.6666700000000043	0.1363000000000008
Fe	Fe34	0.1671948573710769	0.8336760973709337	0.2050156564804286
Fe	Fe35	0.0000441502914627	0.5011826124736301	0.2730100306255474
Fe	Fe36	0.3336810190707846	0.6666729830353886	0.3382638601078052
Fe	Fe37	0.8333300000000222	0.6666700000000282	0.0340699999999998
Fe	Fe38	0.6666700000000044	0.8333299999999968	0.1022200000000026
Fe	Fe39	0.5000000000000036	0.5000000000000033	0.1703699999999984
Fe	Fe40	0.8333366673880638	0.6672524824864375	0.2400563155191833
Fe	Fe41	0.6696335509720391	0.8337121665874638	0.3124054309270982
Fe	Fe42	0.4807802214880477	0.4884411792070473	0.3748818155497514
Fe	Fe43	0.6666700000000044	0.8333299999999968	0.0000000000000000
Fe	Fe44	0.5000000000000036	0.5000000000000033	0.0681500000000028
Fe	Fe45	0.8333300000000222	0.6666700000000282	0.1363000000000008
Fe	Fe46	0.6675419888282584	0.8332898886789284	0.2052317075623474
Fe	Fe47	0.5019092379806877	0.4989859810765569	0.2740754940452295
Fe	Fe48	0.8299551089768507	0.6664722103022710	0.3420821806200161
N	N49	0.2531195426883328	0.2428093325530954	0.4045722297205859
H	H50	0.2621693736172813	0.2148485218688106	0.4462420918135234
H	H51	0.0809810824495892	0.2566950523170650	0.3907466479977009

3.10 H_2N+H hydrogenation.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 8.0101

_cell_length_b 8.0101

_cell_length_c 23.9928

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 120.0000

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.1666700000000037	0.3333300000000039	0.1022200000000026
Fe	Fe3	0.0000000000000000	0.0000000000000000	0.1703699999999984
Fe	Fe4	0.3336827079557435	0.1673710730333430	0.2389071323598994
Fe	Fe5	0.1665145784079122	0.3331111188108321	0.3104735144389876
Fe	Fe6	0.0036897936094763	0.0003461190109232	0.3715049202108321
Fe	Fe7	0.1666700000000037	0.3333300000000039	0.0000000000000000
Fe	Fe8	0.0000000000000000	0.0000000000000000	0.0681500000000028
Fe	Fe9	0.3333299999999971	0.1666700000000036	0.1363000000000017
Fe	Fe10	0.1662439997956262	0.3331672121892963	0.2049489742685748
Fe	Fe11	0.0000363187880471	-0.0011965118979616	0.2733819753058920
Fe	Fe12	0.3334899339135151	0.1668525859037891	0.3389142955212717
Fe	Fe13	0.8333300000000265	0.1666700000000183	0.0340699999999998
Fe	Fe14	0.6666700000000044	0.3333299999999970	0.1022200000000026
Fe	Fe15	0.5000000000000036	-0.0000000000000004	0.1703699999999984
Fe	Fe16	0.8328612117154613	0.1658174111954673	0.2391446686427637
Fe	Fe17	0.6665368388688349	0.3329647933740669	0.3103513016028032
Fe	Fe18	0.4962934577537381	0.0011854113055233	0.3717539786634546
Fe	Fe19	0.6666700000000044	0.3333299999999970	0.0000000000000000
Fe	Fe20	0.5000000000000036	-0.0000000000000004	0.0681500000000028
Fe	Fe21	0.8333300000000265	0.1666700000000183	0.1363000000000017

Fe	Fe22	0.6668906306499452	0.3331611992920561	0.2049294417412929
Fe	Fe23	0.4986188145168312	-0.0012838773019705	0.2734373094353866
Fe	Fe24	0.8323296089363769	0.1649680259391558	0.3390570515184143
Fe	Fe25	0.3333299999999971	0.6666700000000043	0.0340699999999998
Fe	Fe26	0.1666700000000037	0.8333299999999967	0.1022200000000026
Fe	Fe27	0.0000000000000000	0.5000000000000071	0.1703699999999984
Fe	Fe28	0.3336269209023372	0.6657422581721026	0.2394397552433677
Fe	Fe29	0.1655680431272777	0.8311353265212899	0.3113495244334622
Fe	Fe30	-0.0015033909229969	0.4972707118675629	0.3715408042183312
Fe	Fe31	0.1666700000000037	0.8333299999999967	0.0000000000000000
Fe	Fe32	0.0000000000000000	0.5000000000000071	0.0681500000000028
Fe	Fe33	0.3333299999999971	0.6666700000000043	0.1363000000000017
Fe	Fe34	0.1663120215506860	0.8326464229997219	0.2052545172778492
Fe	Fe35	-0.0000416621609753	0.4998746166315462	0.2733661087511755
Fe	Fe36	0.3355216381438538	0.6641305985132573	0.3403198993846021
Fe	Fe37	0.8333300000000265	0.6666700000000252	0.0340699999999998
Fe	Fe38	0.6666700000000044	0.8333299999999968	0.1022200000000026
Fe	Fe39	0.5000000000000036	0.5000000000000033	0.1703699999999984
Fe	Fe40	0.8320379708317495	0.6657174038387271	0.2394017892587468
Fe	Fe41	0.6655152599711116	0.8314006538397474	0.3106043207588320
Fe	Fe42	0.4940580429501821	0.4871902902798428	0.3768953918541225
Fe	Fe43	0.6666700000000044	0.8333299999999968	0.0000000000000000
Fe	Fe44	0.5000000000000036	0.5000000000000033	0.0681500000000028
Fe	Fe45	0.8333300000000265	0.6666700000000252	0.1363000000000017
Fe	Fe46	0.6666820282670056	0.8334204407779695	0.2050021738141161
Fe	Fe47	0.5000599206921906	0.5002822964038447	0.2738886395464094
Fe	Fe48	0.8284390322841014	0.6638706809435693	0.3401076291282153
N	N49	0.4617090284364787	0.4149740639571093	0.4538470056051681
H	H50	0.3861351491328339	0.2540963650282690	0.4091480632009171
H	H51	0.3357908094538585	0.3678040960025702	0.4753780577968401
H	H52	0.5498570204494518	0.3789028667941114	0.4750934104484085

4. (210) surface

4.1 H adsorption.cif

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_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 5.6640
_cell_length_b 12.6651
_cell_length_c 23.8656
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

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Fe	Fe2	0.5849	0.4255	0.0000
Fe	Fe3	0.0849	0.9255	0.0000
Fe	Fe4	0.5849	0.9255	0.0000
Fe	Fe5	0.8349	0.0755	0.0265
Fe	Fe6	0.3349	0.5755	0.0265
Fe	Fe7	0.8349	0.5755	0.0265
Fe	Fe8	0.3349	0.0755	0.0265
Fe	Fe9	0.5849	0.2255	0.0531
Fe	Fe10	0.0849	0.2255	0.0531
Fe	Fe11	0.0849	0.7255	0.0531
Fe	Fe12	0.5849	0.7255	0.0531

Fe	Fe13	0.3349	0.3755	0.0796
Fe	Fe14	0.8349	0.3755	0.0796
Fe	Fe15	0.3349	0.8755	0.0796
Fe	Fe16	0.8349	0.8755	0.0796
Fe	Fe17	0.5849	0.0255	0.1061
Fe	Fe18	0.0849	0.0255	0.1061
Fe	Fe19	0.0849	0.5255	0.1061
Fe	Fe20	0.5849	0.5255	0.1061
Fe	Fe21	0.3349	0.1755	0.1327
Fe	Fe22	0.8349	0.1755	0.1327
Fe	Fe23	0.3349	0.6755	0.1327
Fe	Fe24	0.8349	0.6755	0.1327
Fe	Fe25	0.5849	0.3255	0.1592
Fe	Fe26	0.0849	0.8255	0.1592
Fe	Fe27	0.0849	0.3255	0.1592
Fe	Fe28	0.5849	0.8255	0.1592
Fe	Fe29	0.3349	0.4755	0.1857
Fe	Fe30	0.8349	0.4755	0.1857
Fe	Fe31	0.3349	0.9755	0.1857
Fe	Fe32	0.8349	0.9755	0.1857
Fe	Fe33	0.5849	0.1255	0.2123
Fe	Fe34	0.0849	0.6255	0.2123
Fe	Fe35	0.0849	0.1255	0.2123
Fe	Fe36	0.5849	0.6255	0.2123
Fe	Fe37	0.3349	0.2755	0.2388
Fe	Fe38	0.8349	0.2755	0.2388
Fe	Fe39	0.3349	0.7755	0.2388
Fe	Fe40	0.8349	0.7755	0.2388
Fe	Fe41	0.5849	0.4255	0.2653
Fe	Fe42	0.0849	0.9255	0.2653
Fe	Fe43	0.5849	0.9255	0.2653
Fe	Fe44	0.0849	0.4255	0.2653
Fe	Fe45	0.3348799999999983	0.0771186839430466	0.2914312861786696

Fe	Fe46	0.8348799999999983	0.0771807020019084	0.2912857214869872
Fe	Fe47	0.3348799999999983	0.5774562876350647	0.2914330114224188
Fe	Fe48	0.8348799999999983	0.5765681151845602	0.2918162167889822
Fe	Fe49	0.5836918148885020	0.2276310969153146	0.3208091467581938
Fe	Fe50	0.0842556372920993	0.7261061695158267	0.3213495783809824
Fe	Fe51	0.5855043627078971	0.7261061695158267	0.3213495783809824
Fe	Fe52	0.0860681851114947	0.2276310969153146	0.3208091467581938
Fe	Fe53	0.3348799999999983	0.3807743770728136	0.3471673882817533
Fe	Fe54	0.8348799999999983	0.3798229331836607	0.3464630035002909
Fe	Fe55	0.3348799999999983	0.8796900586194466	0.3463296279992451
Fe	Fe56	0.8348799999999983	0.8801026798069923	0.3462894911959101
Fe	Fe57	0.5854664261512079	0.0341804643729221	0.3682419215321843
Fe	Fe58	0.0814094517314534	0.5340904545429058	0.3694436093421630
Fe	Fe59	0.5883505482685432	0.5340904545429058	0.3694436093421630
Fe	Fe60	0.0842935738487887	0.0341804643729221	0.3682419215321843
H	H61	0.3348769999999988	0.4742253878507546	0.4034960815982577

4.2 N adsorption.cif

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_symmetry_space_group_name_H-M          'P1'
_symmetry_Int_Tables_number             1
_symmetry_cell_setting                  triclinic
loop_
_symmetry_equiv_pos_as_xyz
   x,y,z
_cell_length_a                          5.6640
_cell_length_b                          12.6651
_cell_length_c                          23.8656
_cell_angle_alpha                       90.0000
_cell_angle_beta                        90.0000
_cell_angle_gamma                       90.0000
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loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_U_iso_or_equiv

_atom_site_adp_type

_atom_site_occupancy

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Fe2	Fe	0.58490	0.42550	0.00000	0.00000	Uiso	1.00
Fe3	Fe	0.08490	0.92550	0.00000	0.00000	Uiso	1.00
Fe4	Fe	0.58490	0.92550	0.00000	0.00000	Uiso	1.00
Fe5	Fe	0.83490	0.07550	0.02650	0.00000	Uiso	1.00
Fe6	Fe	0.33490	0.57550	0.02650	0.00000	Uiso	1.00
Fe7	Fe	0.83490	0.57550	0.02650	0.00000	Uiso	1.00
Fe8	Fe	0.33490	0.07550	0.02650	0.00000	Uiso	1.00
Fe9	Fe	0.58490	0.22550	0.05310	0.00000	Uiso	1.00
Fe10	Fe	0.08490	0.22550	0.05310	0.00000	Uiso	1.00
Fe11	Fe	0.08490	0.72550	0.05310	0.00000	Uiso	1.00
Fe12	Fe	0.58490	0.72550	0.05310	0.00000	Uiso	1.00
Fe13	Fe	0.33490	0.37550	0.07960	0.00000	Uiso	1.00
Fe14	Fe	0.83490	0.37550	0.07960	0.00000	Uiso	1.00
Fe15	Fe	0.33490	0.87550	0.07960	0.00000	Uiso	1.00
Fe16	Fe	0.83490	0.87550	0.07960	0.00000	Uiso	1.00
Fe17	Fe	0.58490	0.02550	0.10610	0.00000	Uiso	1.00
Fe18	Fe	0.08490	0.02550	0.10610	0.00000	Uiso	1.00
Fe19	Fe	0.08490	0.52550	0.10610	0.00000	Uiso	1.00
Fe20	Fe	0.58490	0.52550	0.10610	0.00000	Uiso	1.00
Fe21	Fe	0.33490	0.17550	0.13270	0.00000	Uiso	1.00
Fe22	Fe	0.83490	0.17550	0.13270	0.00000	Uiso	1.00
Fe23	Fe	0.33490	0.67550	0.13270	0.00000	Uiso	1.00
Fe24	Fe	0.83490	0.67550	0.13270	0.00000	Uiso	1.00

Fe25	Fe	0.58490	0.32550	0.15920	0.00000	Uiso	1.00
Fe26	Fe	0.08490	0.82550	0.15920	0.00000	Uiso	1.00
Fe27	Fe	0.08490	0.32550	0.15920	0.00000	Uiso	1.00
Fe28	Fe	0.58490	0.82550	0.15920	0.00000	Uiso	1.00
Fe29	Fe	0.33490	0.47550	0.18570	0.00000	Uiso	1.00
Fe30	Fe	0.83490	0.47550	0.18570	0.00000	Uiso	1.00
Fe31	Fe	0.33490	0.97550	0.18570	0.00000	Uiso	1.00
Fe32	Fe	0.83490	0.97550	0.18570	0.00000	Uiso	1.00
Fe33	Fe	0.58490	0.12550	0.21230	0.00000	Uiso	1.00
Fe34	Fe	0.08490	0.62550	0.21230	0.00000	Uiso	1.00
Fe35	Fe	0.08490	0.12550	0.21230	0.00000	Uiso	1.00
Fe36	Fe	0.58490	0.62550	0.21230	0.00000	Uiso	1.00
Fe37	Fe	0.33490	0.27550	0.23880	0.00000	Uiso	1.00
Fe38	Fe	0.83490	0.27550	0.23880	0.00000	Uiso	1.00
Fe39	Fe	0.33490	0.77550	0.23880	0.00000	Uiso	1.00
Fe40	Fe	0.83490	0.77550	0.23880	0.00000	Uiso	1.00
Fe41	Fe	0.58490	0.42550	0.26530	0.00000	Uiso	1.00
Fe42	Fe	0.08490	0.92550	0.26530	0.00000	Uiso	1.00
Fe43	Fe	0.58490	0.92550	0.26530	0.00000	Uiso	1.00
Fe44	Fe	0.08490	0.42550	0.26530	0.00000	Uiso	1.00
Fe45	Fe	0.33490	0.07740	0.29150	0.00000	Uiso	1.00
Fe46	Fe	0.83490	0.07690	0.29140	0.00000	Uiso	1.00
Fe47	Fe	0.33490	0.57300	0.28740	0.00000	Uiso	1.00
Fe48	Fe	0.83490	0.57730	0.29150	0.00000	Uiso	1.00
Fe49	Fe	0.58650	0.22750	0.32090	0.00000	Uiso	1.00
Fe50	Fe	0.09040	0.72560	0.32200	0.00000	Uiso	1.00
Fe51	Fe	0.57940	0.72560	0.32200	0.00000	Uiso	1.00
Fe52	Fe	0.08320	0.22760	0.32100	0.00000	Uiso	1.00
Fe53	Fe	0.33490	0.37950	0.34640	0.00000	Uiso	1.00
Fe54	Fe	0.83480	0.38200	0.34670	0.00000	Uiso	1.00
Fe55	Fe	0.33500	0.88250	0.34610	0.00000	Uiso	1.00
Fe56	Fe	0.83490	0.87850	0.34580	0.00000	Uiso	1.00
Fe57	Fe	0.58500	0.03470	0.36850	0.00000	Uiso	1.00

Fe58 Fe 0.08890 0.53640 0.36850 0.00000 Uiso 1.00

Fe59 Fe 0.58100 0.53640 0.36850 0.00000 Uiso 1.00

Fe60 Fe 0.08490 0.03470 0.36850 0.00000 Uiso 1.00

N61 N 0.33500 0.64250 0.35920 0.00000 Uiso 1.00

4.3 N_2 adsorption.cif

data_

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_cell_length_b 12.6651

_cell_length_c 23.8656

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe Fe1 0.0849 0.4255 0.0000

Fe Fe2 0.5849 0.4255 0.0000

Fe Fe3 0.0849 0.9255 0.0000

Fe Fe4 0.5849 0.9255 0.0000

Fe Fe5 0.8349 0.0755 0.0265

Fe Fe6 0.3349 0.5755 0.0265

Fe Fe7 0.8349 0.5755 0.0265

Fe Fe8 0.3349 0.0755 0.0265

Fe	Fe9	0.5849	0.2255	0.0531
Fe	Fe10	0.0849	0.2255	0.0531
Fe	Fe11	0.0849	0.7255	0.0531
Fe	Fe12	0.5849	0.7255	0.0531
Fe	Fe13	0.3349	0.3755	0.0796
Fe	Fe14	0.8349	0.3755	0.0796
Fe	Fe15	0.3349	0.8755	0.0796
Fe	Fe16	0.8349	0.8755	0.0796
Fe	Fe17	0.5849	0.0255	0.1061
Fe	Fe18	0.0849	0.0255	0.1061
Fe	Fe19	0.0849	0.5255	0.1061
Fe	Fe20	0.5849	0.5255	0.1061
Fe	Fe21	0.3349	0.1755	0.1327
Fe	Fe22	0.8349	0.1755	0.1327
Fe	Fe23	0.3349	0.6755	0.1327
Fe	Fe24	0.8349	0.6755	0.1327
Fe	Fe25	0.5849	0.3255	0.1592
Fe	Fe26	0.0849	0.8255	0.1592
Fe	Fe27	0.0849	0.3255	0.1592
Fe	Fe28	0.5849	0.8255	0.1592
Fe	Fe29	0.3349	0.4755	0.1857
Fe	Fe30	0.8349	0.4755	0.1857
Fe	Fe31	0.3349	0.9755	0.1857
Fe	Fe32	0.8349	0.9755	0.1857
Fe	Fe33	0.5849	0.1255	0.2123
Fe	Fe34	0.0849	0.6255	0.2123
Fe	Fe35	0.0849	0.1255	0.2123
Fe	Fe36	0.5849	0.6255	0.2123
Fe	Fe37	0.3349	0.2755	0.2388
Fe	Fe38	0.8349	0.2755	0.2388
Fe	Fe39	0.3349	0.7755	0.2388
Fe	Fe40	0.8349	0.7755	0.2388
Fe	Fe41	0.5849	0.4255	0.2653

Fe	Fe42	0.0849	0.9255	0.2653
Fe	Fe43	0.5849	0.9255	0.2653
Fe	Fe44	0.0849	0.4255	0.2653
Fe	Fe45	0.3348130112345364	0.0759974479133177	0.2915834447036471
Fe	Fe46	0.8348200296519108	0.0767259022482894	0.2915247130995142
Fe	Fe47	0.3348748446948740	0.5741613030494253	0.2907425137628385
Fe	Fe48	0.8348379099614689	0.5762098331397595	0.2918491425293195
Fe	Fe49	0.5859703623543416	0.2259567523641447	0.3205788876839498
Fe	Fe50	0.0760517121782848	0.7298294006599664	0.3197930025798536
Fe	Fe51	0.5937038336090702	0.7298150830850979	0.3198021990554804
Fe	Fe52	0.0836762846877907	0.2259814543484415	0.3205603092017466
Fe	Fe53	0.3348813607827160	0.3776722111368492	0.3469163676197597
Fe	Fe54	0.8348643883474463	0.3788691443732842	0.3459527336024702
Fe	Fe55	0.3348737473499322	0.8800845574766419	0.3496938895115738
Fe	Fe56	0.8348692130338941	0.8842890752981750	0.3453845919716284
Fe	Fe57	0.5827421251065594	0.0353397598895801	0.3690087350573811
Fe	Fe58	0.0784099456663295	0.5300183981117098	0.3704900162641511
Fe	Fe59	0.5912871574659261	0.5299988574948765	0.3704941438514008
Fe	Fe60	0.0868585692274189	0.0352949275319336	0.3690063712222427
N	N61	0.3349055874438014	0.6312646338163871	0.3796888743253811
N	N62	0.3348563407807187	0.7341427282071724	0.3766096295249722

4.4 NH adsorption.cif

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_cell_angle_gamma 90.0000

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loop_

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_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.5849	0.4255	0.0000
Fe	Fe3	0.0849	0.9255	0.0000
Fe	Fe4	0.5849	0.9255	0.0000
Fe	Fe5	0.8349	0.0755	0.0265
Fe	Fe6	0.3349	0.5755	0.0265
Fe	Fe7	0.8349	0.5755	0.0265
Fe	Fe8	0.3349	0.0755	0.0265
Fe	Fe9	0.5849	0.2255	0.0531
Fe	Fe10	0.0849	0.2255	0.0531
Fe	Fe11	0.0849	0.7255	0.0531
Fe	Fe12	0.5849	0.7255	0.0531
Fe	Fe13	0.3349	0.3755	0.0796
Fe	Fe14	0.8349	0.3755	0.0796
Fe	Fe15	0.3349	0.8755	0.0796
Fe	Fe16	0.8349	0.8755	0.0796
Fe	Fe17	0.5849	0.0255	0.1061
Fe	Fe18	0.0849	0.0255	0.1061
Fe	Fe19	0.0849	0.5255	0.1061
Fe	Fe20	0.5849	0.5255	0.1061
Fe	Fe21	0.3349	0.1755	0.1327
Fe	Fe22	0.8349	0.1755	0.1327
Fe	Fe23	0.3349	0.6755	0.1327
Fe	Fe24	0.8349	0.6755	0.1327

Fe	Fe25	0.5849	0.3255	0.1592
Fe	Fe26	0.0849	0.8255	0.1592
Fe	Fe27	0.0849	0.3255	0.1592
Fe	Fe28	0.5849	0.8255	0.1592
Fe	Fe29	0.3349	0.4755	0.1857
Fe	Fe30	0.8349	0.4755	0.1857
Fe	Fe31	0.3349	0.9755	0.1857
Fe	Fe32	0.8349	0.9755	0.1857
Fe	Fe33	0.5849	0.1255	0.2123
Fe	Fe34	0.0849	0.6255	0.2123
Fe	Fe35	0.0849	0.1255	0.2123
Fe	Fe36	0.5849	0.6255	0.2123
Fe	Fe37	0.3349	0.2755	0.2388
Fe	Fe38	0.8349	0.2755	0.2388
Fe	Fe39	0.3349	0.7755	0.2388
Fe	Fe40	0.8349	0.7755	0.2388
Fe	Fe41	0.5849	0.4255	0.2653
Fe	Fe42	0.0849	0.9255	0.2653
Fe	Fe43	0.5849	0.9255	0.2653
Fe	Fe44	0.0849	0.4255	0.2653
Fe	Fe45	0.3348799999999983	0.0767653841663170	0.2912129596342167
Fe	Fe46	0.8348799999999983	0.0768210621590371	0.2910494009250505
Fe	Fe47	0.3348799999999983	0.5774692111211593	0.2911669823784253
Fe	Fe48	0.8348799999999983	0.5770855191769449	0.2907280566669769
Fe	Fe49	0.5835560705189001	0.2267169868602738	0.3207864696199693
Fe	Fe50	0.0831397694368621	0.7257089658911365	0.3211759706850493
Fe	Fe51	0.5866202305631339	0.7257089658911365	0.3211759706850493
Fe	Fe52	0.0862039294810968	0.2267169868602738	0.3207864696199693
Fe	Fe53	0.3348799999999983	0.3780179497684071	0.3472627342768262
Fe	Fe54	0.8348799999999983	0.3811173763179521	0.3448042916342524
Fe	Fe55	0.3348799999999983	0.8790635478527533	0.3463330052397418
Fe	Fe56	0.8348799999999983	0.8802008585626411	0.3463316725445023
Fe	Fe57	0.5851895172107564	0.0339356162686215	0.3679556003488349

Fe	Fe58	0.0735417833476838	0.5365368498042185	0.3702507154898719
Fe	Fe59	0.5962182166523127	0.5365368498042185	0.3702507154898719
Fe	Fe60	0.0845704827892400	0.0339356162686215	0.3679556003488349
N	N61	0.3348769999999988	0.4753762219043642	0.4083363323819811
H	H62	0.3348769999999988	0.4522847417337336	0.4497007038965254

4.5 NH_2 adsorption.cif

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_cell_length_c          23.8656
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_cell_angle_beta           90.0000
_cell_angle_gamma          90.0000

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loop_
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_atom_site_label
_atom_site_fract_x
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_atom_site_fract_z
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Fe      Fe2             0.5849      0.4255      0.0000
Fe      Fe3             0.0849      0.9255      0.0000
Fe      Fe4             0.5849      0.9255      0.0000
Fe      Fe5             0.8349      0.0755      0.0265
Fe      Fe6             0.3349      0.5755      0.0265
Fe      Fe7             0.8349      0.5755      0.0265
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Fe	Fe8	0.3349	0.0755	0.0265
Fe	Fe9	0.5849	0.2255	0.0531
Fe	Fe10	0.0849	0.2255	0.0531
Fe	Fe11	0.0849	0.7255	0.0531
Fe	Fe12	0.5849	0.7255	0.0531
Fe	Fe13	0.3349	0.3755	0.0796
Fe	Fe14	0.8349	0.3755	0.0796
Fe	Fe15	0.3349	0.8755	0.0796
Fe	Fe16	0.8349	0.8755	0.0796
Fe	Fe17	0.5849	0.0255	0.1061
Fe	Fe18	0.0849	0.0255	0.1061
Fe	Fe19	0.0849	0.5255	0.1061
Fe	Fe20	0.5849	0.5255	0.1061
Fe	Fe21	0.3349	0.1755	0.1327
Fe	Fe22	0.8349	0.1755	0.1327
Fe	Fe23	0.3349	0.6755	0.1327
Fe	Fe24	0.8349	0.6755	0.1327
Fe	Fe25	0.5849	0.3255	0.1592
Fe	Fe26	0.0849	0.8255	0.1592
Fe	Fe27	0.0849	0.3255	0.1592
Fe	Fe28	0.5849	0.8255	0.1592
Fe	Fe29	0.3349	0.4755	0.1857
Fe	Fe30	0.8349	0.4755	0.1857
Fe	Fe31	0.3349	0.9755	0.1857
Fe	Fe32	0.8349	0.9755	0.1857
Fe	Fe33	0.5849	0.1255	0.2123
Fe	Fe34	0.0849	0.6255	0.2123
Fe	Fe35	0.0849	0.1255	0.2123
Fe	Fe36	0.5849	0.6255	0.2123
Fe	Fe37	0.3349	0.2755	0.2388
Fe	Fe38	0.8349	0.2755	0.2388
Fe	Fe39	0.3349	0.7755	0.2388
Fe	Fe40	0.8349	0.7755	0.2388

Fe	Fe41	0.5849	0.4255	0.2653
Fe	Fe42	0.0849	0.9255	0.2653
Fe	Fe43	0.5849	0.9255	0.2653
Fe	Fe44	0.0849	0.4255	0.2653
Fe	Fe45	0.3348110950258772	0.0768785197798810	0.2914078227861046
Fe	Fe46	0.8348127874067083	0.0767289364027657	0.2913284392234624
Fe	Fe47	0.3348377983227757	0.5766229273569019	0.2913052074029543
Fe	Fe48	0.8348522918742262	0.5757901770861847	0.2921114695938085
Fe	Fe49	0.5861895532120047	0.2263368020909879	0.3209936472574478
Fe	Fe50	0.0824053415971532	0.7255711285556437	0.3203536688228441
Fe	Fe51	0.5871429133525683	0.7255427427245945	0.3203662480593669
Fe	Fe52	0.0834064149205911	0.2263543472960766	0.3209827958316333
Fe	Fe53	0.3349169585925639	0.3775735932871454	0.3444006609496363
Fe	Fe54	0.8348623856413002	0.3812190661661448	0.3462862345022213
Fe	Fe55	0.3348131930226969	0.8789984798566981	0.3460060918108075
Fe	Fe56	0.8347821412035097	0.8793262336109881	0.3463082917127538
Fe	Fe57	0.5845713237811073	0.0331500829163105	0.3681749360806446
Fe	Fe58	0.0902983998435851	0.5349453575367860	0.3716472426128533
Fe	Fe59	0.5794762713641339	0.5349677159708374	0.3716637939919064
Fe	Fe60	0.0850973075904245	0.0331513044038065	0.3681671946655229
N	N61	0.3348217208204110	0.5456033594028366	0.4316220619399597
H	H62	0.3347904237409045	0.4878072796137878	0.4616853222244935
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4.6 NH_3 adsorption.cif

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loop_

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Fe	Fe3	0.0849	0.9255	0.0000
Fe	Fe4	0.5849	0.9255	0.0000
Fe	Fe5	0.8349	0.0755	0.0265
Fe	Fe6	0.3349	0.5755	0.0265
Fe	Fe7	0.8349	0.5755	0.0265
Fe	Fe8	0.3349	0.0755	0.0265
Fe	Fe9	0.5849	0.2255	0.0531
Fe	Fe10	0.0849	0.2255	0.0531
Fe	Fe11	0.0849	0.7255	0.0531
Fe	Fe12	0.5849	0.7255	0.0531
Fe	Fe13	0.3349	0.3755	0.0796
Fe	Fe14	0.8349	0.3755	0.0796
Fe	Fe15	0.3349	0.8755	0.0796
Fe	Fe16	0.8349	0.8755	0.0796
Fe	Fe17	0.5849	0.0255	0.1061
Fe	Fe18	0.0849	0.0255	0.1061
Fe	Fe19	0.0849	0.5255	0.1061
Fe	Fe20	0.5849	0.5255	0.1061
Fe	Fe21	0.3349	0.1755	0.1327
Fe	Fe22	0.8349	0.1755	0.1327

Fe	Fe23	0.3349	0.6755	0.1327
Fe	Fe24	0.8349	0.6755	0.1327
Fe	Fe25	0.5849	0.3255	0.1592
Fe	Fe26	0.0849	0.8255	0.1592
Fe	Fe27	0.0849	0.3255	0.1592
Fe	Fe28	0.5849	0.8255	0.1592
Fe	Fe29	0.3349	0.4755	0.1857
Fe	Fe30	0.8349	0.4755	0.1857
Fe	Fe31	0.3349	0.9755	0.1857
Fe	Fe32	0.8349	0.9755	0.1857
Fe	Fe33	0.5849	0.1255	0.2123
Fe	Fe34	0.0849	0.6255	0.2123
Fe	Fe35	0.0849	0.1255	0.2123
Fe	Fe36	0.5849	0.6255	0.2123
Fe	Fe37	0.3349	0.2755	0.2388
Fe	Fe38	0.8349	0.2755	0.2388
Fe	Fe39	0.3349	0.7755	0.2388
Fe	Fe40	0.8349	0.7755	0.2388
Fe	Fe41	0.5849	0.4255	0.2653
Fe	Fe42	0.0849	0.9255	0.2653
Fe	Fe43	0.5849	0.9255	0.2653
Fe	Fe44	0.0849	0.4255	0.2653
Fe	Fe45	0.3348411558782651	0.0768472823266639	0.2915140187352369
Fe	Fe46	0.8348018783448988	0.0768427592148157	0.2915134756193694
Fe	Fe47	0.3377759472910357	0.5770376801284901	0.2910666554404133
Fe	Fe48	0.8318065762277174	0.5770352464296049	0.2910552630190253
Fe	Fe49	0.5848218268318108	0.2267999598775596	0.3211857227778538
Fe	Fe50	0.0847610516969839	0.7267054883191845	0.3210393633578035
Fe	Fe51	0.5848238574372923	0.7269725334663368	0.3210985975599712
Fe	Fe52	0.0848236193018746	0.2267360197584591	0.3213093070022550
Fe	Fe53	0.3357481488002948	0.3796881910882215	0.3461739101717474
Fe	Fe54	0.8337952264354003	0.3796929805048496	0.3461966213440451
Fe	Fe55	0.3346531085036467	0.8794402929656713	0.3465034352249241

Fe	Fe56	0.8349233113092468	0.8794395740409441	0.3465083057621694
Fe	Fe57	0.5847794484259101	0.0333483646261997	0.3684258891484365
Fe	Fe58	0.0845012325875878	0.5331874141453723	0.3658009764060934
Fe	Fe59	0.5847433657661767	0.5346603985454241	0.3714463181162383
Fe	Fe60	0.0847817471122329	0.0333553184168350	0.3684632144312036
N	N61	0.5810843688397943	0.5677653412321156	0.4587302892052676
H	H62	0.5812038199376468	0.4996008056573970	0.4818850315209621
H	H63	0.4339133635307335	0.6107976722330331	0.4689950794473010
H	H64	0.7260287806115741	0.6117333965657636	0.4696460912821051

4.7 N_2 activation.cif

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x,y,z

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loop_

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Fe4	Fe	0.58490	0.92550	0.00000	0.00000	Uiso	1.00
Fe5	Fe	0.83490	0.07550	0.02650	0.00000	Uiso	1.00
Fe6	Fe	0.33490	0.57550	0.02650	0.00000	Uiso	1.00
Fe7	Fe	0.83490	0.57550	0.02650	0.00000	Uiso	1.00
Fe8	Fe	0.33490	0.07550	0.02650	0.00000	Uiso	1.00
Fe9	Fe	0.58490	0.22550	0.05310	0.00000	Uiso	1.00
Fe10	Fe	0.08490	0.22550	0.05310	0.00000	Uiso	1.00
Fe11	Fe	0.08490	0.72550	0.05310	0.00000	Uiso	1.00
Fe12	Fe	0.58490	0.72550	0.05310	0.00000	Uiso	1.00
Fe13	Fe	0.33490	0.37550	0.07960	0.00000	Uiso	1.00
Fe14	Fe	0.83490	0.37550	0.07960	0.00000	Uiso	1.00
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Fe16	Fe	0.83490	0.87550	0.07960	0.00000	Uiso	1.00
Fe17	Fe	0.58490	0.02550	0.10610	0.00000	Uiso	1.00
Fe18	Fe	0.08490	0.02550	0.10610	0.00000	Uiso	1.00
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Fe20	Fe	0.58490	0.52550	0.10610	0.00000	Uiso	1.00
Fe21	Fe	0.33490	0.17550	0.13270	0.00000	Uiso	1.00
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Fe23	Fe	0.33490	0.67550	0.13270	0.00000	Uiso	1.00
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Fe26	Fe	0.08490	0.82550	0.15920	0.00000	Uiso	1.00
Fe27	Fe	0.08490	0.32550	0.15920	0.00000	Uiso	1.00
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Fe29	Fe	0.33490	0.47550	0.18570	0.00000	Uiso	1.00
Fe30	Fe	0.83490	0.47550	0.18570	0.00000	Uiso	1.00
Fe31	Fe	0.33490	0.97550	0.18570	0.00000	Uiso	1.00

Fe32	Fe	0.83490	0.97550	0.18570	0.00000	Uiso	1.00
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Fe34	Fe	0.08490	0.62550	0.21230	0.00000	Uiso	1.00
Fe35	Fe	0.08490	0.12550	0.21230	0.00000	Uiso	1.00
Fe36	Fe	0.58490	0.62550	0.21230	0.00000	Uiso	1.00
Fe37	Fe	0.33490	0.27550	0.23880	0.00000	Uiso	1.00
Fe38	Fe	0.83490	0.27550	0.23880	0.00000	Uiso	1.00
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Fe42	Fe	0.08490	0.92550	0.26530	0.00000	Uiso	1.00
Fe43	Fe	0.58490	0.92550	0.26530	0.00000	Uiso	1.00
Fe44	Fe	0.08490	0.42550	0.26530	0.00000	Uiso	1.00
Fe45	Fe	0.33490	0.07690	0.29110	0.00000	Uiso	1.00
Fe46	Fe	0.83490	0.07700	0.29120	0.00000	Uiso	1.00
Fe47	Fe	0.33490	0.57440	0.29090	0.00000	Uiso	1.00
Fe48	Fe	0.83490	0.57660	0.29170	0.00000	Uiso	1.00
Fe49	Fe	0.58430	0.22560	0.32030	0.00000	Uiso	1.00
Fe50	Fe	0.08400	0.72980	0.32180	0.00000	Uiso	1.00
Fe51	Fe	0.58580	0.72980	0.32180	0.00000	Uiso	1.00
Fe52	Fe	0.08540	0.22560	0.32030	0.00000	Uiso	1.00
Fe53	Fe	0.33490	0.37630	0.34700	0.00000	Uiso	1.00
Fe54	Fe	0.83490	0.37540	0.34530	0.00000	Uiso	1.00
Fe55	Fe	0.33490	0.88870	0.34800	0.00000	Uiso	1.00
Fe56	Fe	0.83490	0.88400	0.34550	0.00000	Uiso	1.00
Fe57	Fe	0.58560	0.03780	0.36890	0.00000	Uiso	1.00
Fe58	Fe	0.07010	0.52620	0.37000	0.00000	Uiso	1.00
Fe59	Fe	0.59970	0.52620	0.37000	0.00000	Uiso	1.00
Fe60	Fe	0.08420	0.03780	0.36890	0.00000	Uiso	1.00
N61	N	0.33490	0.61220	0.37000	0.00000	Uiso	1.00
N62	N	0.33490	0.75290	0.37170	0.00000	Uiso	1.00

4.8 N+H hydrogenation.cif

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_cell_length_c          23.8656
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_cell_angle_beta          90.0000
_cell_angle_gamma          90.0000

_symmetry_space_group_name_H-M    'T'

loop_
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_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
Fe     Fe1            0.0849     0.4255     0.0000
Fe     Fe2            0.5849     0.4255     0.0000
Fe     Fe3            0.0849     0.9255     0.0000
Fe     Fe4            0.5849     0.9255     0.0000
Fe     Fe5            0.8349     0.0755     0.0265
Fe     Fe6            0.3349     0.5755     0.0265
Fe     Fe7            0.8349     0.5755     0.0265
Fe     Fe8            0.3349     0.0755     0.0265
Fe     Fe9            0.5849     0.2255     0.0531
Fe     Fe10           0.0849     0.2255     0.0531
Fe     Fe11           0.0849     0.7255     0.0531
Fe     Fe12           0.5849     0.7255     0.0531
Fe     Fe13           0.3349     0.3755     0.0796
Fe     Fe14           0.8349     0.3755     0.0796
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Fe	Fe15	0.3349	0.8755	0.0796
Fe	Fe16	0.8349	0.8755	0.0796
Fe	Fe17	0.5849	0.0255	0.1061
Fe	Fe18	0.0849	0.0255	0.1061
Fe	Fe19	0.0849	0.5255	0.1061
Fe	Fe20	0.5849	0.5255	0.1061
Fe	Fe21	0.3349	0.1755	0.1327
Fe	Fe22	0.8349	0.1755	0.1327
Fe	Fe23	0.3349	0.6755	0.1327
Fe	Fe24	0.8349	0.6755	0.1327
Fe	Fe25	0.5849	0.3255	0.1592
Fe	Fe26	0.0849	0.8255	0.1592
Fe	Fe27	0.0849	0.3255	0.1592
Fe	Fe28	0.5849	0.8255	0.1592
Fe	Fe29	0.3349	0.4755	0.1857
Fe	Fe30	0.8349	0.4755	0.1857
Fe	Fe31	0.3349	0.9755	0.1857
Fe	Fe32	0.8349	0.9755	0.1857
Fe	Fe33	0.5849	0.1255	0.2123
Fe	Fe34	0.0849	0.6255	0.2123
Fe	Fe35	0.0849	0.1255	0.2123
Fe	Fe36	0.5849	0.6255	0.2123
Fe	Fe37	0.3349	0.2755	0.2388
Fe	Fe38	0.8349	0.2755	0.2388
Fe	Fe39	0.3349	0.7755	0.2388
Fe	Fe40	0.8349	0.7755	0.2388
Fe	Fe41	0.5849	0.4255	0.2653
Fe	Fe42	0.0849	0.9255	0.2653
Fe	Fe43	0.5849	0.9255	0.2653
Fe	Fe44	0.0849	0.4255	0.2653
Fe	Fe45	0.3347724921188569	0.0774862109831898	0.2913835940908724
Fe	Fe46	0.8347708434781596	0.0768698251224578	0.2916059650318437
Fe	Fe47	0.3348240538872108	0.5746556032332918	0.2891034603470812

Fe	Fe48	0.8348137100212851	0.5762671935246043	0.2915615869640319
Fe	Fe49	0.5859783774172161	0.2271603025373916	0.3208332842661534
Fe	Fe50	0.0829390404775730	0.7273112018141432	0.3222358982811040
Fe	Fe51	0.5865913705154971	0.7272907790102788	0.3222425056814784
Fe	Fe52	0.0835309337254560	0.2271452363347932	0.3208311822154720
Fe	Fe53	0.3348155597831001	0.3784936400951098	0.3464880503430494
Fe	Fe54	0.8347647436495145	0.3799871993745388	0.3464005065238960
Fe	Fe55	0.3347619054192708	0.8841217175077382	0.3452717383954244
Fe	Fe56	0.8347287547618490	0.8807012876591422	0.3465990153536209
Fe	Fe57	0.5834003453968080	0.0362121952859238	0.3688444271125583
Fe	Fe58	0.0830825241978168	0.5327289668915850	0.3688689672602959
Fe	Fe59	0.5864992247128884	0.5327630309862136	0.3688645722022033
Fe	Fe60	0.0859695802272007	0.0362195227223735	0.3688377639551292
N	N61	0.3347952589652414	0.6356891297218707	0.3649593366564901
H	H62	0.3347226465978875	0.7405947300349054	0.3730192207921884

4.9 HN+H hydrogenation.cif

data_

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_cell_length_c 23.8656
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_
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_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.5849	0.4255	0.0000
Fe	Fe3	0.0849	0.9255	0.0000
Fe	Fe4	0.5849	0.9255	0.0000
Fe	Fe5	0.8349	0.0755	0.0265
Fe	Fe6	0.3349	0.5755	0.0265
Fe	Fe7	0.8349	0.5755	0.0265
Fe	Fe8	0.3349	0.0755	0.0265
Fe	Fe9	0.5849	0.2255	0.0531
Fe	Fe10	0.0849	0.2255	0.0531
Fe	Fe11	0.0849	0.7255	0.0531
Fe	Fe12	0.5849	0.7255	0.0531
Fe	Fe13	0.3349	0.3755	0.0796
Fe	Fe14	0.8349	0.3755	0.0796
Fe	Fe15	0.3349	0.8755	0.0796
Fe	Fe16	0.8349	0.8755	0.0796
Fe	Fe17	0.5849	0.0255	0.1061
Fe	Fe18	0.0849	0.0255	0.1061
Fe	Fe19	0.0849	0.5255	0.1061
Fe	Fe20	0.5849	0.5255	0.1061
Fe	Fe21	0.3349	0.1755	0.1327
Fe	Fe22	0.8349	0.1755	0.1327
Fe	Fe23	0.3349	0.6755	0.1327
Fe	Fe24	0.8349	0.6755	0.1327
Fe	Fe25	0.5849	0.3255	0.1592
Fe	Fe26	0.0849	0.8255	0.1592
Fe	Fe27	0.0849	0.3255	0.1592
Fe	Fe28	0.5849	0.8255	0.1592
Fe	Fe29	0.3349	0.4755	0.1857
Fe	Fe30	0.8349	0.4755	0.1857

Fe	Fe31	0.3349	0.9755	0.1857
Fe	Fe32	0.8349	0.9755	0.1857
Fe	Fe33	0.5849	0.1255	0.2123
Fe	Fe34	0.0849	0.6255	0.2123
Fe	Fe35	0.0849	0.1255	0.2123
Fe	Fe36	0.5849	0.6255	0.2123
Fe	Fe37	0.3349	0.2755	0.2388
Fe	Fe38	0.8349	0.2755	0.2388
Fe	Fe39	0.3349	0.7755	0.2388
Fe	Fe40	0.8349	0.7755	0.2388
Fe	Fe41	0.5849	0.4255	0.2653
Fe	Fe42	0.0849	0.9255	0.2653
Fe	Fe43	0.5849	0.9255	0.2653
Fe	Fe44	0.0849	0.4255	0.2653
Fe	Fe45	0.3344869508799533	0.0769424455376115	0.2911603980707477
Fe	Fe46	0.8343197519092326	0.0767221373840908	0.2910040238584132
Fe	Fe47	0.3364034591214916	0.5773936260740088	0.2913924028267740
Fe	Fe48	0.8387617703111165	0.5774377235042470	0.2914220224475698
Fe	Fe49	0.5819651335171273	0.2266576582637489	0.3210532638993585
Fe	Fe50	0.0850383311370693	0.7259901263765403	0.3213574253745068
Fe	Fe51	0.5862847798718223	0.7269003642164177	0.3205105789819065
Fe	Fe52	0.0823093945004178	0.2263277937648004	0.3208499619729714
Fe	Fe53	0.3272726891400270	0.3760653334886440	0.3468747791225224
Fe	Fe54	0.8302587544170805	0.3813377996042424	0.3461037371583767
Fe	Fe55	0.3349439853540434	0.8798059057005110	0.3464425946852970
Fe	Fe56	0.8346213934486247	0.8805017288910706	0.3463763835210760
Fe	Fe57	0.5856613109085752	0.0342034595282807	0.3679067919619236
Fe	Fe58	0.0833142295758939	0.5330853080496809	0.3709727766825010
Fe	Fe59	0.6047359153635407	0.5426512847396679	0.3706648120021945
Fe	Fe60	0.0845119498032474	0.0341456985569406	0.3679981660390806
N	N61	0.3477045626677011	0.4754497721947308	0.4137105192998859
H	H62	0.5342085784733105	0.4109666187031378	0.4001439945755169
H	H63	0.3398108680206347	0.4584917062535384	0.4557541000490694

4.10 H_2N+H hydrogenation.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 5.6640
_cell_length_b 12.6651
_cell_length_c 23.8656
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

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Fe	Fe2	0.5849	0.4255	0.0000
Fe	Fe3	0.0849	0.9255	0.0000
Fe	Fe4	0.5849	0.9255	0.0000
Fe	Fe5	0.8349	0.0755	0.0265
Fe	Fe6	0.3349	0.5755	0.0265
Fe	Fe7	0.8349	0.5755	0.0265
Fe	Fe8	0.3349	0.0755	0.0265
Fe	Fe9	0.5849	0.2255	0.0531
Fe	Fe10	0.0849	0.2255	0.0531
Fe	Fe11	0.0849	0.7255	0.0531
Fe	Fe12	0.5849	0.7255	0.0531

Fe	Fe13	0.3349	0.3755	0.0796
Fe	Fe14	0.8349	0.3755	0.0796
Fe	Fe15	0.3349	0.8755	0.0796
Fe	Fe16	0.8349	0.8755	0.0796
Fe	Fe17	0.5849	0.0255	0.1061
Fe	Fe18	0.0849	0.0255	0.1061
Fe	Fe19	0.0849	0.5255	0.1061
Fe	Fe20	0.5849	0.5255	0.1061
Fe	Fe21	0.3349	0.1755	0.1327
Fe	Fe22	0.8349	0.1755	0.1327
Fe	Fe23	0.3349	0.6755	0.1327
Fe	Fe24	0.8349	0.6755	0.1327
Fe	Fe25	0.5849	0.3255	0.1592
Fe	Fe26	0.0849	0.8255	0.1592
Fe	Fe27	0.0849	0.3255	0.1592
Fe	Fe28	0.5849	0.8255	0.1592
Fe	Fe29	0.3349	0.4755	0.1857
Fe	Fe30	0.8349	0.4755	0.1857
Fe	Fe31	0.3349	0.9755	0.1857
Fe	Fe32	0.8349	0.9755	0.1857
Fe	Fe33	0.5849	0.1255	0.2123
Fe	Fe34	0.0849	0.6255	0.2123
Fe	Fe35	0.0849	0.1255	0.2123
Fe	Fe36	0.5849	0.6255	0.2123
Fe	Fe37	0.3349	0.2755	0.2388
Fe	Fe38	0.8349	0.2755	0.2388
Fe	Fe39	0.3349	0.7755	0.2388
Fe	Fe40	0.8349	0.7755	0.2388
Fe	Fe41	0.5849	0.4255	0.2653
Fe	Fe42	0.0849	0.9255	0.2653
Fe	Fe43	0.5849	0.9255	0.2653
Fe	Fe44	0.0849	0.4255	0.2653
Fe	Fe45	0.3345987704330990	0.0769921259539278	0.2914025222834047

Fe	Fe46	0.8344200718231365	0.0767046367603630	0.2912848922764969
Fe	Fe47	0.3325641109742660	0.5770919625752334	0.2904400010389893
Fe	Fe48	0.8361199077054120	0.5757593814824234	0.2924622947015398
Fe	Fe49	0.5869878532626487	0.2267642899428228	0.3211360230469303
Fe	Fe50	0.0822904671620259	0.7256562365955070	0.3208665285498596
Fe	Fe51	0.5858659931018875	0.7253661843946617	0.3204777294085669
Fe	Fe52	0.0813774406059841	0.2264410620113241	0.3209540117003785
Fe	Fe53	0.3325492984476407	0.3768540944839930	0.3440963865202917
Fe	Fe54	0.8340984765158252	0.3820122681424869	0.3474660556869568
Fe	Fe55	0.3345318678743616	0.8791046487953500	0.3461041049688854
Fe	Fe56	0.8339521211850014	0.8792909845448139	0.3463590073664961
Fe	Fe57	0.5843137725710483	0.0334683484068484	0.3681699489780779
Fe	Fe58	0.0988415307847036	0.5360727777225782	0.3727966434540355
Fe	Fe59	0.5769207736035865	0.5338452294511780	0.3688530353110770
Fe	Fe60	0.0849232038299269	0.0333148530910868	0.3681114956076985
N	N61	0.3462821232356805	0.5411049858744548	0.4373277086326686
H	H62	0.5935961021431813	0.5273533631098578	0.4369123508578753
H	H63	0.3146057317585411	0.4809177920189465	0.4650983183389116
H	H64	0.3368774473903129	0.6113208569942626	0.4588523745503150

5. (211) surface

5.1 H adsorption.cif

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_cell_length_b 8.0101

_cell_length_c 24.2493

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.6937	0.0323	0.0000
Fe	Fe3	0.1937	0.5323	0.0000
Fe	Fe4	0.1937	0.0323	0.0000
Fe	Fe5	0.3604	0.2823	0.0477
Fe	Fe6	0.8604	0.7823	0.0477
Fe	Fe7	0.3604	0.7823	0.0477
Fe	Fe8	0.8604	0.2823	0.0477
Fe	Fe9	0.0271	0.5323	0.0954
Fe	Fe10	0.0271	0.0323	0.0954
Fe	Fe11	0.5271	0.0323	0.0954
Fe	Fe12	0.5271	0.5323	0.0954
Fe	Fe13	0.1937	0.7823	0.1430
Fe	Fe14	0.1937	0.2823	0.1430
Fe	Fe15	0.6937	0.2823	0.1430
Fe	Fe16	0.6937	0.7823	0.1430
Fe	Fe17	0.8604	0.5323	0.1907
Fe	Fe18	0.8604	0.0323	0.1907
Fe	Fe19	0.3604	0.5323	0.1907
Fe	Fe20	0.3604	0.0323	0.1907
Fe	Fe21	0.0271	0.7823	0.2384
Fe	Fe22	0.5271	0.7823	0.2384
Fe	Fe23	0.0271	0.2823	0.2384
Fe	Fe24	0.5271	0.2823	0.2384

Fe	Fe25	0.6951750770413426	0.0321621246662703	0.2861845522848783
Fe	Fe26	0.1944661661610134	0.0325623994495705	0.2863373146893277
Fe	Fe27	0.1944661661610134	0.5320141615464673	0.2863373146893277
Fe	Fe28	0.6951750770413426	0.5324144363297676	0.2861845522848783
Fe	Fe29	0.8553451894113497	0.7822880069062705	0.3360255520595545
Fe	Fe30	0.8572560257238281	0.2822882804356013	0.3370254182587480
Fe	Fe31	0.3527907529778380	0.2822882804356013	0.3364314660777170
Fe	Fe32	0.3566269467544258	0.7822880069062705	0.3363509508943604
Fe	Fe33	0.5515597118950496	0.0318312695041917	0.3794692679540162
Fe	Fe34	0.0537123387297124	0.0283773411962839	0.3804970254077953
Fe	Fe35	0.5515597118950496	0.5327452914918461	0.3794692679540162
Fe	Fe36	0.0537123387297124	0.5361992197997539	0.3804970254077953
H	H37	0.5996421225850049	0.2822878454852713	0.3888807424559234

5.2 N adsorption.cif

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_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.1937	0.5323	0.0000
Fe	Fe2	0.6937	0.0323	0.0000
Fe	Fe3	0.1937	0.0323	0.0000
Fe	Fe4	0.6937	0.5323	0.0000
Fe	Fe5	0.8604	0.7823	0.0477
Fe	Fe6	0.3604	0.2823	0.0477
Fe	Fe7	0.8604	0.2823	0.0477
Fe	Fe8	0.3604	0.7823	0.0477
Fe	Fe9	0.0271	0.0323	0.0954
Fe	Fe10	0.0271	0.5323	0.0954
Fe	Fe11	0.5271	0.0323	0.0954
Fe	Fe12	0.5271	0.5323	0.0954
Fe	Fe13	0.1937	0.2823	0.1430
Fe	Fe14	0.6937	0.7823	0.1430
Fe	Fe15	0.1937	0.7823	0.1430
Fe	Fe16	0.6937	0.2823	0.1430
Fe	Fe17	0.8604	0.5323	0.1907
Fe	Fe18	0.3604	0.5323	0.1907
Fe	Fe19	0.8604	0.0323	0.1907
Fe	Fe20	0.3604	0.0323	0.1907
Fe	Fe21	0.5271	0.7823	0.2384
Fe	Fe22	0.5271	0.2823	0.2384
Fe	Fe23	0.0271	0.7823	0.2384
Fe	Fe24	0.0271	0.2823	0.2384
Fe	Fe25	0.6953	0.0312	0.2870
Fe	Fe26	0.1957	0.0299	0.2863
Fe	Fe27	0.1957	0.5347	0.2863
Fe	Fe28	0.6953	0.5334	0.2870
Fe	Fe29	0.8535	0.7823	0.3365
Fe	Fe30	0.8584	0.2823	0.3358
Fe	Fe31	0.3382	0.2823	0.3332
Fe	Fe32	0.3603	0.7823	0.3386

Fe	Fe33	0.5550	0.0469	0.3831
Fe	Fe34	0.0567	0.0216	0.3789
Fe	Fe35	0.5550	0.5177	0.3831
Fe	Fe36	0.0567	0.5430	0.3789
N	N37	0.5891	0.2823	0.3907

5.3 N_2 adsorption.cif

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_cell_length_c 24.2493
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_cell_angle_beta 90.0000
_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

Fe	Fe1	0.6937	0.5323	0.0000
Fe	Fe2	0.6937	0.0323	0.0000
Fe	Fe3	0.1937	0.5323	0.0000
Fe	Fe4	0.1937	0.0323	0.0000
Fe	Fe5	0.3604	0.2823	0.0477
Fe	Fe6	0.8604	0.7823	0.0477
Fe	Fe7	0.3604	0.7823	0.0477

Fe	Fe8	0.8604	0.2823	0.0477
Fe	Fe9	0.0271	0.5323	0.0954
Fe	Fe10	0.0271	0.0323	0.0954
Fe	Fe11	0.5271	0.0323	0.0954
Fe	Fe12	0.5271	0.5323	0.0954
Fe	Fe13	0.1937	0.7823	0.1430
Fe	Fe14	0.1937	0.2823	0.1430
Fe	Fe15	0.6937	0.2823	0.1430
Fe	Fe16	0.6937	0.7823	0.1430
Fe	Fe17	0.8604	0.5323	0.1907
Fe	Fe18	0.8604	0.0323	0.1907
Fe	Fe19	0.3604	0.5323	0.1907
Fe	Fe20	0.3604	0.0323	0.1907
Fe	Fe21	0.0271	0.7823	0.2384
Fe	Fe22	0.5271	0.7823	0.2384
Fe	Fe23	0.0271	0.2823	0.2384
Fe	Fe24	0.5271	0.2823	0.2384
Fe	Fe25	0.6944217669482858	0.0293200703003628	0.2867410219766325
Fe	Fe26	0.1939040199937689	0.0292603525275779	0.2864433268285339
Fe	Fe27	0.1938912098132445	0.5353766306257493	0.2864231449411377
Fe	Fe28	0.6944201594076180	0.5353441998141670	0.2867181889688619
Fe	Fe29	0.8539728324179097	0.7823961472625013	0.3390845779181207
Fe	Fe30	0.8529424423634926	0.2824417093329461	0.3326846903921361
Fe	Fe31	0.3611911981284734	0.2823859868177016	0.3322340089859803
Fe	Fe32	0.3559799961202711	0.7823560811528808	0.3386449596760415
Fe	Fe33	0.5611747797178875	0.0367383685796443	0.3831601041697688
Fe	Fe34	0.0497673128110318	0.0422327381399567	0.3803207900515830
Fe	Fe35	0.5612611221817848	0.5280295752563205	0.3831360819281150
Fe	Fe36	0.0497332037918491	0.5226852373722987	0.3803013673777935
N	N37	0.3017081941371835	0.2011001659524531	0.4122403579712550
N	N38	0.3017528410403110	0.3639175970173350	0.4122378917334784

5.4 NH adsorption.cif

data_

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_cell_length_b 8.0101
_cell_length_c 24.2493
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

Fe	Fe1	0.6937	0.5323	0.0000
Fe	Fe2	0.6937	0.0323	0.0000
Fe	Fe3	0.1937	0.5323	0.0000
Fe	Fe4	0.1937	0.0323	0.0000
Fe	Fe5	0.3604	0.2823	0.0477
Fe	Fe6	0.8604	0.7823	0.0477
Fe	Fe7	0.3604	0.7823	0.0477
Fe	Fe8	0.8604	0.2823	0.0477
Fe	Fe9	0.0271	0.5323	0.0954
Fe	Fe10	0.0271	0.0323	0.0954
Fe	Fe11	0.5271	0.0323	0.0954
Fe	Fe12	0.5271	0.5323	0.0954
Fe	Fe13	0.1937	0.7823	0.1430
Fe	Fe14	0.1937	0.2823	0.1430

Fe Fe15 0.6937 0.2823 0.1430

Fe Fe16 0.6937 0.7823 0.1430

Fe Fe17 0.8604 0.5323 0.1907

Fe Fe18 0.8604 0.0323 0.1907

Fe Fe19 0.3604 0.5323 0.1907

Fe Fe20 0.3604 0.0323 0.1907

Fe Fe21 0.0271 0.7823 0.2384

Fe Fe22 0.5271 0.7823 0.2384

Fe Fe23 0.0271 0.2823 0.2384

Fe Fe24 0.5271 0.2823 0.2384

Fe Fe25 0.6946137579984083 0.0326224226461234 0.2859110753026053

Fe Fe26 0.1963405051456390 0.0338411587161757 0.2861783956751181

Fe Fe27 0.1955934137577052 0.5317265589408836 0.2859834572242427

Fe Fe28 0.6954175118419368 0.5320080721041917 0.2857950538545829

Fe Fe29 0.8561828189991095 0.7817398697242913 0.3350127637770033

Fe Fe30 0.8546033071136793 0.2814815049007510 0.3352044579315868

Fe Fe31 0.3592866209474344 0.2821239744985432 0.3412045032912648

Fe Fe32 0.3557682151732889 0.7817768881366549 0.3353412677523888

Fe Fe33 0.5519508669478707 0.0245340883929974 0.3796640159255915

Fe Fe34 0.0468002300050003 0.0256676318181722 0.3781819130304946

Fe Fe35 0.5667968645240082 0.5420498161803842 0.3796085658505088

Fe Fe36 0.0425646971502717 0.5357761904449659 0.3779748147674155

N N37 0.3093683095385608 0.4040049253791311 0.4110644623303524

H H38 0.3067784606318057 0.3481683187504234 0.4491428759110015

5.5 NH_2 adsorption.cif

data_

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_cell_length_b 8.0101

_cell_length_c 24.2493

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.6937	0.0323	0.0000
Fe	Fe3	0.1937	0.5323	0.0000
Fe	Fe4	0.1937	0.0323	0.0000
Fe	Fe5	0.3604	0.2823	0.0477
Fe	Fe6	0.8604	0.7823	0.0477
Fe	Fe7	0.3604	0.7823	0.0477
Fe	Fe8	0.8604	0.2823	0.0477
Fe	Fe9	0.0271	0.5323	0.0954
Fe	Fe10	0.0271	0.0323	0.0954
Fe	Fe11	0.5271	0.0323	0.0954
Fe	Fe12	0.5271	0.5323	0.0954
Fe	Fe13	0.1937	0.7823	0.1430
Fe	Fe14	0.1937	0.2823	0.1430
Fe	Fe15	0.6937	0.2823	0.1430
Fe	Fe16	0.6937	0.7823	0.1430
Fe	Fe17	0.8604	0.5323	0.1907
Fe	Fe18	0.8604	0.0323	0.1907
Fe	Fe19	0.3604	0.5323	0.1907
Fe	Fe20	0.3604	0.0323	0.1907
Fe	Fe21	0.0271	0.7823	0.2384

Fe	Fe22	0.5271	0.7823	0.2384
Fe	Fe23	0.0271	0.2823	0.2384
Fe	Fe24	0.5271	0.2823	0.2384
Fe	Fe25	0.6950094009868253	0.0322664256702878	0.2860646597327205
Fe	Fe26	0.1943582329981497	0.0322703068737692	0.2859074746579243
Fe	Fe27	0.1935860653196854	0.5322541339862085	0.2865759256416903
Fe	Fe28	0.6938217246046933	0.5322593274692569	0.2872818729725685
Fe	Fe29	0.8539428613771383	0.7805776797911081	0.3363123240461242
Fe	Fe30	0.8539251313756470	0.2838955417082755	0.3363139228703365
Fe	Fe31	0.3539218274025070	0.2819576222355011	0.3355053495406089
Fe	Fe32	0.3539373134598577	0.7825318868921316	0.3354961417288330
Fe	Fe33	0.5499889730802046	0.0322506273992440	0.3790598316288989
Fe	Fe34	0.0513554612830495	0.0322261958246737	0.3792833917784583
Fe	Fe35	0.5500437346976127	0.5322682643380849	0.3817937165444556
Fe	Fe36	0.0518668362390324	0.5322314976730478	0.3818643072850073
N	N37	0.2996123922905481	0.5323762152689034	0.4453275224953903
H	H38	0.3036800999935560	0.6368032874851247	0.4696715339286998
H	H39	0.3037142546718318	0.4281181812051052	0.4697435419040646

5.6 NH_3 adsorption.cif

data_

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_cell_length_b 8.0101
_cell_length_c 24.2493
_cell_angle_alpha 90.0000
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_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

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_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
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Fe  Fe2  0.6937  0.0323  0.0000
Fe  Fe3  0.1937  0.5323  0.0000
Fe  Fe4  0.1937  0.0323  0.0000
Fe  Fe5  0.3604  0.2823  0.0477
Fe  Fe6  0.8604  0.7823  0.0477
Fe  Fe7  0.3604  0.7823  0.0477
Fe  Fe8  0.8604  0.2823  0.0477
Fe  Fe9  0.0271  0.5323  0.0954
Fe  Fe10  0.0271  0.0323  0.0954
Fe  Fe11  0.5271  0.0323  0.0954
Fe  Fe12  0.5271  0.5323  0.0954
Fe  Fe13  0.1937  0.7823  0.1430
Fe  Fe14  0.1937  0.2823  0.1430
Fe  Fe15  0.6937  0.2823  0.1430
Fe  Fe16  0.6937  0.7823  0.1430
Fe  Fe17  0.8604  0.5323  0.1907
Fe  Fe18  0.8604  0.0323  0.1907
Fe  Fe19  0.3604  0.5323  0.1907
Fe  Fe20  0.3604  0.0323  0.1907
Fe  Fe21  0.0271  0.7823  0.2384
Fe  Fe22  0.5271  0.7823  0.2384
Fe  Fe23  0.0271  0.2823  0.2384
Fe  Fe24  0.5271  0.2823  0.2384
Fe  Fe25  0.6931614331119388  0.0322646087289459  0.2864703522780309
Fe  Fe26  0.1939086676726191  0.0322789775593663  0.2863330423541458
Fe  Fe27  0.1942783812761952  0.5322684997641394  0.2859933841431362
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Fe	Fe28	0.6924796027948289	0.5322786689265036	0.2868267581800954
Fe	Fe29	0.8530797359289768	0.7825511511699144	0.3359729029921402
Fe	Fe30	0.8531124587872680	0.2820021999154799	0.3359631438929705
Fe	Fe31	0.3535179100535844	0.2829339352804119	0.3369015919844396
Fe	Fe32	0.3535364408593088	0.7815254868365304	0.3369122169551058
Fe	Fe33	0.5508434333843669	0.0322575427780920	0.3804471507098531
Fe	Fe34	0.0495502368635151	0.0323204442619353	0.3795299515153904
Fe	Fe35	0.5557539055481056	0.5322791818403628	0.3842543517896850
Fe	Fe36	0.0473614432159943	0.5322986017019194	0.3773712256491294
N	N37	0.5226621731964955	0.5316054184991933	0.4712445647121353
H	H38	0.7118728041717884	0.5323750688439440	0.4891578560564793
H	H39	0.4209969321032637	0.4262062068465347	0.4835688520525675
H	H40	0.4184457493798602	0.6358901751530710	0.4837536543873291

5.7 N_2 activation.cif

data_

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_cell_length_a 4.9052
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_cell_length_c 24.2493
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
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_atom_site_fract_z

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Fe	Fe2	0.6937	0.0323	0.0000
Fe	Fe3	0.1937	0.5323	0.0000
Fe	Fe4	0.1937	0.0323	0.0000
Fe	Fe5	0.3604	0.2823	0.0477
Fe	Fe6	0.8604	0.7823	0.0477
Fe	Fe7	0.3604	0.7823	0.0477
Fe	Fe8	0.8604	0.2823	0.0477
Fe	Fe9	0.0271	0.5323	0.0954
Fe	Fe10	0.0271	0.0323	0.0954
Fe	Fe11	0.5271	0.0323	0.0954
Fe	Fe12	0.5271	0.5323	0.0954
Fe	Fe13	0.1937	0.7823	0.1430
Fe	Fe14	0.1937	0.2823	0.1430
Fe	Fe15	0.6937	0.2823	0.1430
Fe	Fe16	0.6937	0.7823	0.1430
Fe	Fe17	0.8604	0.5323	0.1907
Fe	Fe18	0.8604	0.0323	0.1907
Fe	Fe19	0.3604	0.5323	0.1907
Fe	Fe20	0.3604	0.0323	0.1907
Fe	Fe21	0.0271	0.7823	0.2384
Fe	Fe22	0.5271	0.7823	0.2384
Fe	Fe23	0.0271	0.2823	0.2384
Fe	Fe24	0.5271	0.2823	0.2384
Fe	Fe25	0.6941	0.0304	0.2863
Fe	Fe26	0.1940	0.5339	0.2859
Fe	Fe27	0.6941	0.5341	0.2863
Fe	Fe28	0.1940	0.0306	0.2859
Fe	Fe29	0.3569	0.7821	0.3375
Fe	Fe30	0.3597	0.2822	0.3363
Fe	Fe31	0.8517	0.2823	0.3336
Fe	Fe32	0.8566	0.7822	0.3373

Fe Fe33 0.0473 0.0374 0.3786

Fe Fe34 0.5643 0.0265 0.3816

Fe Fe35 0.5645 0.5377 0.3816

Fe Fe36 0.0476 0.5270 0.3786

N N37 0.3085 0.1704 0.4081

N N38 0.3086 0.3936 0.4081

5.8 N+H hydrogenation.cif

data_

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_cell_length_b 8.0101

_cell_length_c 24.2493

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_

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_atom_site_label

_atom_site_fract_x

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_atom_site_fract_z

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Fe Fe2 0.6937 0.0323 0.0000

Fe Fe3 0.1937 0.5323 0.0000

Fe Fe4 0.1937 0.0323 0.0000

Fe Fe5 0.3604 0.2823 0.0477

Fe Fe6 0.8604 0.7823 0.0477

Fe	Fe7	0.3604	0.7823	0.0477
Fe	Fe8	0.8604	0.2823	0.0477
Fe	Fe9	0.0271	0.5323	0.0954
Fe	Fe10	0.0271	0.0323	0.0954
Fe	Fe11	0.5271	0.0323	0.0954
Fe	Fe12	0.5271	0.5323	0.0954
Fe	Fe13	0.1937	0.7823	0.1430
Fe	Fe14	0.1937	0.2823	0.1430
Fe	Fe15	0.6937	0.2823	0.1430
Fe	Fe16	0.6937	0.7823	0.1430
Fe	Fe17	0.8604	0.5323	0.1907
Fe	Fe18	0.8604	0.0323	0.1907
Fe	Fe19	0.3604	0.5323	0.1907
Fe	Fe20	0.3604	0.0323	0.1907
Fe	Fe21	0.0271	0.7823	0.2384
Fe	Fe22	0.5271	0.7823	0.2384
Fe	Fe23	0.0271	0.2823	0.2384
Fe	Fe24	0.5271	0.2823	0.2384
Fe	Fe25	0.6942277911241097	0.0321179729759762	0.2861556856740901
Fe	Fe26	0.1952834810755946	0.0325881427750115	0.2862002965509537
Fe	Fe27	0.1953285234751136	0.5330662176453509	0.2856586716396947
Fe	Fe28	0.6958288109040005	0.5329019587866687	0.2861759179418214
Fe	Fe29	0.8574082557344570	0.7822640885854243	0.3360114745096644
Fe	Fe30	0.8537131546679473	0.2817887529146021	0.3348309558725201
Fe	Fe31	0.3590054738947119	0.2828597012292679	0.3395070400601417
Fe	Fe32	0.3564584934197059	0.7822947651853112	0.3358111101466568
Fe	Fe33	0.5495237795781985	0.0272001821750234	0.3797472883039523
Fe	Fe34	0.0483940167504381	0.0280110116074358	0.3792610095335567
Fe	Fe35	0.5685097255322008	0.5436347474333035	0.3803583993574455
Fe	Fe36	0.0512715699872950	0.5326428665140082	0.3782634221276358
N	N37	0.3166538594232345	0.4082180608722711	0.4095958225042839
H	H38	0.3251619044865465	0.2296577186398075	0.4072017258158122

5.9 HN+H hydrogenation.cif

data_

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_cell_length_c 24.2493
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
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_atom_site_fract_z

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Fe	Fe2	0.6937	0.0323	0.0000
Fe	Fe3	0.1937	0.5323	0.0000
Fe	Fe4	0.1937	0.0323	0.0000
Fe	Fe5	0.3604	0.2823	0.0477
Fe	Fe6	0.8604	0.7823	0.0477
Fe	Fe7	0.3604	0.7823	0.0477
Fe	Fe8	0.8604	0.2823	0.0477
Fe	Fe9	0.0271	0.5323	0.0954
Fe	Fe10	0.0271	0.0323	0.0954
Fe	Fe11	0.5271	0.0323	0.0954
Fe	Fe12	0.5271	0.5323	0.0954
Fe	Fe13	0.1937	0.7823	0.1430

Fe	Fe14	0.1937	0.2823	0.1430
Fe	Fe15	0.6937	0.2823	0.1430
Fe	Fe16	0.6937	0.7823	0.1430
Fe	Fe17	0.8604	0.5323	0.1907
Fe	Fe18	0.8604	0.0323	0.1907
Fe	Fe19	0.3604	0.5323	0.1907
Fe	Fe20	0.3604	0.0323	0.1907
Fe	Fe21	0.0271	0.7823	0.2384
Fe	Fe22	0.5271	0.7823	0.2384
Fe	Fe23	0.0271	0.2823	0.2384
Fe	Fe24	0.5271	0.2823	0.2384
Fe	Fe25	0.6928378331019239	0.0329378785578832	0.2862774368542735
Fe	Fe26	0.1937025307698975	0.0318539069926775	0.2861793186302038
Fe	Fe27	0.1927320425153511	0.5322027703994572	0.2863782115043270
Fe	Fe28	0.6920169078575155	0.5320183536188375	0.2862277871580292
Fe	Fe29	0.8490135019290553	0.7824043819773924	0.3349305044312133
Fe	Fe30	0.8530844688002397	0.2835879911615991	0.3356614109876153
Fe	Fe31	0.3526054189064632	0.2828772603842736	0.3357970701995689
Fe	Fe32	0.3536590237877900	0.7831780982191329	0.3384246502961042
Fe	Fe33	0.5458197542741035	0.0376260180790314	0.3796403034423933
Fe	Fe34	0.0431419372812499	0.0375337386219326	0.3790416471556675
Fe	Fe35	0.5595392583385366	0.5229359232050087	0.3811688400070308
Fe	Fe36	0.0396189147512864	0.5295743625343924	0.3788135809164220
N	N37	0.2997855060756421	0.6546678989792141	0.4188377829683299
H	H38	0.2980511344032529	0.8283034942521664	0.4067653252798571
H	H39	0.2973925429723009	0.6771700996525228	0.4605940756787784

5.10 H_2N+H hydrogenation.cif

data_

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_cell_length_c 24.2493

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 90.0000

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.6937	0.0323	0.0000
Fe	Fe3	0.1937	0.5323	0.0000
Fe	Fe4	0.1937	0.0323	0.0000
Fe	Fe5	0.3604	0.2823	0.0477
Fe	Fe6	0.8604	0.7823	0.0477
Fe	Fe7	0.3604	0.7823	0.0477
Fe	Fe8	0.8604	0.2823	0.0477
Fe	Fe9	0.0271	0.5323	0.0954
Fe	Fe10	0.0271	0.0323	0.0954
Fe	Fe11	0.5271	0.0323	0.0954
Fe	Fe12	0.5271	0.5323	0.0954
Fe	Fe13	0.1937	0.7823	0.1430
Fe	Fe14	0.1937	0.2823	0.1430
Fe	Fe15	0.6937	0.2823	0.1430
Fe	Fe16	0.6937	0.7823	0.1430
Fe	Fe17	0.8604	0.5323	0.1907
Fe	Fe18	0.8604	0.0323	0.1907
Fe	Fe19	0.3604	0.5323	0.1907

Fe	Fe20	0.3604	0.0323	0.1907
Fe	Fe21	0.0271	0.7823	0.2384
Fe	Fe22	0.5271	0.7823	0.2384
Fe	Fe23	0.0271	0.2823	0.2384
Fe	Fe24	0.5271	0.2823	0.2384
Fe	Fe25	0.6922042879900114	0.0323301887811876	0.2861250664158791
Fe	Fe26	0.1938058497156300	0.0323249026225893	0.2860750960972639
Fe	Fe27	0.1943027155119944	0.5323278939298334	0.2862940579108124
Fe	Fe28	0.6896229648344648	0.5323667152539702	0.2875479226190636
Fe	Fe29	0.8488838682983703	0.7827110058884688	0.3354392056782511
Fe	Fe30	0.8489431340379995	0.2820629381024946	0.3354091333899932
Fe	Fe31	0.3502028398923601	0.2852112304284667	0.3368509862284788
Fe	Fe32	0.3501307176590896	0.7795312131027690	0.3368715782782405
Fe	Fe33	0.5471359922767984	0.0324863849698155	0.3800823674745686
Fe	Fe34	0.0455643806779139	0.0324606471056282	0.3781945793972406
Fe	Fe35	0.5423186198617017	0.5324503174594063	0.3865867962110445
Fe	Fe36	0.0453659576984131	0.5324153220256349	0.3773975515154805
N	N37	0.8328671870134996	0.5320028260498046	0.4506121307690011
H	H38	0.1068318918115406	0.5320734065038368	0.4444201990818951
H	H39	0.8130859876322024	0.4272507042553073	0.4745398039624159
H	H40	0.8131405507431205	0.6363752887759196	0.4747219014764171

6. (221) surface

6.1 H adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 8.0101

_cell_length_b 12.6651

_cell_length_c 22.0800

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 108.4350

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.0871	0.1870	0.0000
Fe	Fe3	0.5871	0.6870	0.0000
Fe	Fe4	0.0871	0.6870	0.0000
Fe	Fe5	0.2815	0.5759	0.0214
Fe	Fe6	0.7815	0.5759	0.0214
Fe	Fe7	0.2815	0.0759	0.0214
Fe	Fe8	0.7815	0.0759	0.0214
Fe	Fe9	0.9760	0.9648	0.0428
Fe	Fe10	0.9760	0.4648	0.0428
Fe	Fe11	0.4760	0.9648	0.0428
Fe	Fe12	0.4760	0.4648	0.0428
Fe	Fe13	0.6704	0.8537	0.0641
Fe	Fe14	0.6704	0.3537	0.0641
Fe	Fe15	0.1704	0.8537	0.0641
Fe	Fe16	0.1704	0.3537	0.0641
Fe	Fe17	0.8649	0.7426	0.0855
Fe	Fe18	0.3649	0.7426	0.0855
Fe	Fe19	0.8649	0.2426	0.0855
Fe	Fe20	0.3649	0.2426	0.0855
Fe	Fe21	0.0593	0.6315	0.1069
Fe	Fe22	0.5593	0.6315	0.1069

Fe	Fe23	0.0593	0.1315	0.1069
Fe	Fe24	0.5593	0.1315	0.1069
Fe	Fe25	0.2538	0.0204	0.1283
Fe	Fe26	0.2538	0.5204	0.1283
Fe	Fe27	0.7538	0.5204	0.1283
Fe	Fe28	0.7538	0.0204	0.1283
Fe	Fe29	0.4482	0.4092	0.1496
Fe	Fe30	0.9482	0.4092	0.1496
Fe	Fe31	0.4482	0.9093	0.1496
Fe	Fe32	0.9482	0.9093	0.1496
Fe	Fe33	0.6427	0.2981	0.1710
Fe	Fe34	0.1427	0.2981	0.1710
Fe	Fe35	0.1427	0.7981	0.1710
Fe	Fe36	0.6427	0.7981	0.1710
Fe	Fe37	0.8371	0.6870	0.1924
Fe	Fe38	0.3371	0.1870	0.1924
Fe	Fe39	0.3371	0.6870	0.1924
Fe	Fe40	0.8371	0.1870	0.1924
Fe	Fe41	0.5313883464291238	0.5757743601780573	0.2144975171572270
Fe	Fe42	0.5317047204842805	0.0759375438596005	0.2144521302392641
Fe	Fe43	0.0311917336895436	0.0760569570924845	0.2146312834242043
Fe	Fe44	0.0317266585575427	0.5760979262729151	0.2144237415953116
Fe	Fe45	0.7260977951174872	0.4635846676495299	0.2400835210140654
Fe	Fe46	0.7248569555932660	0.9630003508808893	0.2405971315430374
Fe	Fe47	0.2249787302935413	0.9632087653731661	0.2403182839741904
Fe	Fe48	0.2254495520311580	0.4630429063874151	0.2402295027485532
Fe	Fe49	0.4191038544494495	0.8511943503207875	0.2555072010198415
Fe	Fe50	0.4205742967726819	0.3521374680378611	0.2569397585818634
Fe	Fe51	0.9191980443956551	0.3513978708032650	0.2555429512242238
Fe	Fe52	0.9193703593282173	0.8512008853536228	0.2554901723581093
Fe	Fe53	0.6158110450252252	0.7444062643853421	0.2803624524602704
Fe	Fe54	0.1139369856056057	0.2447914079531550	0.2799818565881240
Fe	Fe55	0.1159718395418033	0.7449841114813285	0.2802198021169483

Fe Fe56 0.6165400768319249 0.2445864234734717 0.2800115131872984

Fe Fe57 0.3122520192322685 0.6381094470583210 0.2993610460435217

Fe Fe58 0.8132036379568359 0.6379606302546650 0.2993932512219733

Fe Fe59 0.8119165516165745 0.1376685418866297 0.2997088013526923

Fe Fe60 0.3121561346835491 0.1375205486873300 0.2990878210956074

Fe Fe61 0.5047821811115640 0.5233080074369870 0.3160258186210133

Fe Fe62 0.0046218199616895 0.0198098546598015 0.3153644923439902

Fe Fe63 0.0045517781251998 0.5210352329605956 0.3156099536290113

Fe Fe64 0.5022886228854759 0.0201230800604790 0.3153871788794830

H H65 0.4388031365751903 0.2755192642499797 0.3211750129139904

6.2 N adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 8.0101

_cell_length_b 12.6651

_cell_length_c 22.0800

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 108.4350

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe Fe2 0.0871 0.1870 0.0000

Fe	Fe3	0.5871	0.6870	0.0000
Fe	Fe4	0.0871	0.6870	0.0000
Fe	Fe5	0.2815	0.5759	0.0214
Fe	Fe6	0.7815	0.5759	0.0214
Fe	Fe7	0.2815	0.0759	0.0214
Fe	Fe8	0.7815	0.0759	0.0214
Fe	Fe9	0.9760	0.9648	0.0428
Fe	Fe10	0.9760	0.4648	0.0428
Fe	Fe11	0.4760	0.9648	0.0428
Fe	Fe12	0.4760	0.4648	0.0428
Fe	Fe13	0.6704	0.8537	0.0641
Fe	Fe14	0.6704	0.3537	0.0641
Fe	Fe15	0.1704	0.8537	0.0641
Fe	Fe16	0.1704	0.3537	0.0641
Fe	Fe17	0.8649	0.7426	0.0855
Fe	Fe18	0.3649	0.7426	0.0855
Fe	Fe19	0.8649	0.2426	0.0855
Fe	Fe20	0.3649	0.2426	0.0855
Fe	Fe21	0.0593	0.6315	0.1069
Fe	Fe22	0.5593	0.6315	0.1069
Fe	Fe23	0.0593	0.1315	0.1069
Fe	Fe24	0.5593	0.1315	0.1069
Fe	Fe25	0.2538	0.0204	0.1283
Fe	Fe26	0.2538	0.5204	0.1283
Fe	Fe27	0.7538	0.5204	0.1283
Fe	Fe28	0.7538	0.0204	0.1283
Fe	Fe29	0.4482	0.4092	0.1496
Fe	Fe30	0.9482	0.4092	0.1496
Fe	Fe31	0.4482	0.9093	0.1496
Fe	Fe32	0.9482	0.9093	0.1496
Fe	Fe33	0.6427	0.2981	0.1710
Fe	Fe34	0.1427	0.2981	0.1710
Fe	Fe35	0.1427	0.7981	0.1710

Fe	Fe36	0.6427	0.7981	0.1710
Fe	Fe37	0.8371	0.6870	0.1924
Fe	Fe38	0.3371	0.1870	0.1924
Fe	Fe39	0.3371	0.6870	0.1924
Fe	Fe40	0.8371	0.1870	0.1924
Fe	Fe41	0.5318	0.5768	0.2146
Fe	Fe42	0.5311	0.0748	0.2176
Fe	Fe43	0.0319	0.0765	0.2152
Fe	Fe44	0.0320	0.5768	0.2146
Fe	Fe45	0.7265	0.4659	0.2404
Fe	Fe46	0.7258	0.9623	0.2413
Fe	Fe47	0.2239	0.9623	0.2413
Fe	Fe48	0.2258	0.4643	0.2406
Fe	Fe49	0.4171	0.8470	0.2523
Fe	Fe50	0.4164	0.3528	0.2557
Fe	Fe51	0.9240	0.3527	0.2557
Fe	Fe52	0.9197	0.8520	0.2565
Fe	Fe53	0.6158	0.7459	0.2810
Fe	Fe54	0.1150	0.2419	0.2811
Fe	Fe55	0.1171	0.7459	0.2809
Fe	Fe56	0.6259	0.2639	0.2771
Fe	Fe57	0.3131	0.6395	0.2998
Fe	Fe58	0.8134	0.6400	0.3000
Fe	Fe59	0.8010	0.1379	0.2996
Fe	Fe60	0.3250	0.1378	0.2996
Fe	Fe61	0.5045	0.5228	0.3158
Fe	Fe62	0.0073	0.0266	0.3167
Fe	Fe63	0.0050	0.5228	0.3157
Fe	Fe64	0.4866	-0.0162	0.3216
N	N65	0.5618	0.1356	0.3199

6.3 N_2 adsorption.cif

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_cell_length_c 22.0800
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 108.4350

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
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_atom_site_fract_z

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Fe	Fe2	0.0871	0.1870	0.0000
Fe	Fe3	0.5871	0.6870	0.0000
Fe	Fe4	0.0871	0.6870	0.0000
Fe	Fe5	0.2815	0.5759	0.0214
Fe	Fe6	0.7815	0.5759	0.0214
Fe	Fe7	0.2815	0.0759	0.0214
Fe	Fe8	0.7815	0.0759	0.0214
Fe	Fe9	0.9760	0.9648	0.0428
Fe	Fe10	0.9760	0.4648	0.0428
Fe	Fe11	0.4760	0.9648	0.0428
Fe	Fe12	0.4760	0.4648	0.0428
Fe	Fe13	0.6704	0.8537	0.0641
Fe	Fe14	0.6704	0.3537	0.0641
Fe	Fe15	0.1704	0.8537	0.0641

Fe	Fe16	0.1704	0.3537	0.0641
Fe	Fe17	0.8649	0.7426	0.0855
Fe	Fe18	0.3649	0.7426	0.0855
Fe	Fe19	0.8649	0.2426	0.0855
Fe	Fe20	0.3649	0.2426	0.0855
Fe	Fe21	0.0593	0.6315	0.1069
Fe	Fe22	0.5593	0.6315	0.1069
Fe	Fe23	0.0593	0.1315	0.1069
Fe	Fe24	0.5593	0.1315	0.1069
Fe	Fe25	0.2538	0.0204	0.1283
Fe	Fe26	0.2538	0.5204	0.1283
Fe	Fe27	0.7538	0.5204	0.1283
Fe	Fe28	0.7538	0.0204	0.1283
Fe	Fe29	0.4482	0.4092	0.1496
Fe	Fe30	0.9482	0.4092	0.1496
Fe	Fe31	0.4482	0.9093	0.1496
Fe	Fe32	0.9482	0.9093	0.1496
Fe	Fe33	0.6427	0.2981	0.1710
Fe	Fe34	0.1427	0.2981	0.1710
Fe	Fe35	0.1427	0.7981	0.1710
Fe	Fe36	0.6427	0.7981	0.1710
Fe	Fe37	0.8371	0.6870	0.1924
Fe	Fe38	0.3371	0.1870	0.1924
Fe	Fe39	0.3371	0.6870	0.1924
Fe	Fe40	0.8371	0.1870	0.1924
Fe	Fe41	0.5302888346296708	0.5762774888197226	0.2150085164406305
Fe	Fe42	0.5322387316398952	0.0771211281923195	0.2150062080691334
Fe	Fe43	0.0316320997792843	0.0751412246428182	0.2144449118627706
Fe	Fe44	0.0341903987741943	0.5768593855658799	0.2145941464086097
Fe	Fe45	0.7242515982042421	0.4638728493178350	0.2350639170454541
Fe	Fe46	0.7253204509629255	0.9623243221543391	0.2398913311459868
Fe	Fe47	0.2257340298176627	0.9627601551587379	0.2405390654954424
Fe	Fe48	0.2246806063397161	0.4629198343394323	0.2408849440610878

Fe	Fe49	0.4207088847402270	0.8512394553815904	0.2557714359713092
Fe	Fe50	0.4148014358755461	0.3500694126353719	0.2550874388888597
Fe	Fe51	0.9225424529386055	0.3520721421423405	0.2578143214513345
Fe	Fe52	0.9195717548459545	0.8498268680628367	0.2561177520129293
Fe	Fe53	0.6180819931014929	0.7463529047629825	0.2805411675756698
Fe	Fe54	0.1148031781262384	0.2429832267096708	0.2793994114644255
Fe	Fe55	0.1195985834431530	0.7452102514236219	0.2808731981998210
Fe	Fe56	0.6170839460906710	0.2461817281921290	0.2823412487366115
Fe	Fe57	0.3145770045458163	0.6358031885374698	0.2997893468477154
Fe	Fe58	0.8145230690162814	0.6388023872720420	0.2988189768152192
Fe	Fe59	0.8124675336610411	0.1357402861694613	0.2988872199222692
Fe	Fe60	0.3143140749349521	0.1388624883288709	0.2993444816028231
Fe	Fe61	0.5081158324853240	0.5170323674060164	0.3167393106314719
Fe	Fe62	0.0056776025278035	0.0203673944035213	0.3154778213222895
Fe	Fe63	0.0118635737489992	0.5267055781368903	0.3178851807719847
Fe	Fe64	0.5025089139948378	0.0213723391046654	0.3158074828255095
N	N65	0.7561352930613023	0.3900082839078829	0.3153917904675795
N	N66	0.7290275884200721	0.4839454712120971	0.3327954619027081

6.4 NH adsorption.cif

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_cell_length_b 12.6651
_cell_length_c 22.0800
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 108.4350

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe3	0.5871	0.6870	0.0000
Fe	Fe4	0.0871	0.6870	0.0000
Fe	Fe5	0.2815	0.5759	0.0214
Fe	Fe6	0.7815	0.5759	0.0214
Fe	Fe7	0.2815	0.0759	0.0214
Fe	Fe8	0.7815	0.0759	0.0214
Fe	Fe9	0.9760	0.9648	0.0428
Fe	Fe10	0.9760	0.4648	0.0428
Fe	Fe11	0.4760	0.9648	0.0428
Fe	Fe12	0.4760	0.4648	0.0428
Fe	Fe13	0.6704	0.8537	0.0641
Fe	Fe14	0.6704	0.3537	0.0641
Fe	Fe15	0.1704	0.8537	0.0641
Fe	Fe16	0.1704	0.3537	0.0641
Fe	Fe17	0.8649	0.7426	0.0855
Fe	Fe18	0.3649	0.7426	0.0855
Fe	Fe19	0.8649	0.2426	0.0855
Fe	Fe20	0.3649	0.2426	0.0855
Fe	Fe21	0.0593	0.6315	0.1069
Fe	Fe22	0.5593	0.6315	0.1069
Fe	Fe23	0.0593	0.1315	0.1069
Fe	Fe24	0.5593	0.1315	0.1069
Fe	Fe25	0.2538	0.0204	0.1283
Fe	Fe26	0.2538	0.5204	0.1283
Fe	Fe27	0.7538	0.5204	0.1283

Fe	Fe28	0.7538	0.0204	0.1283
Fe	Fe29	0.4482	0.4092	0.1496
Fe	Fe30	0.9482	0.4092	0.1496
Fe	Fe31	0.4482	0.9093	0.1496
Fe	Fe32	0.9482	0.9093	0.1496
Fe	Fe33	0.6427	0.2981	0.1710
Fe	Fe34	0.1427	0.2981	0.1710
Fe	Fe35	0.1427	0.7981	0.1710
Fe	Fe36	0.6427	0.7981	0.1710
Fe	Fe37	0.8371	0.6870	0.1924
Fe	Fe38	0.3371	0.1870	0.1924
Fe	Fe39	0.3371	0.6870	0.1924
Fe	Fe40	0.8371	0.1870	0.1924
Fe	Fe41	0.5317297349104686	0.5763467077591039	0.2145814085531314
Fe	Fe42	0.5307635061597921	0.0743388273690835	0.2140388828830745
Fe	Fe43	0.0320045620602477	0.0768242802625440	0.2148741139132501
Fe	Fe44	0.0317048186322423	0.5763465174244417	0.2145794363126859
Fe	Fe45	0.7256731396556493	0.4641123355787950	0.2400566355564555
Fe	Fe46	0.7254451608755030	0.9630700917632966	0.2409070628269374
Fe	Fe47	0.2248939051337245	0.9630783201640287	0.2409170596324008
Fe	Fe48	0.2250613817456270	0.4628980895449862	0.2404415713767249
Fe	Fe49	0.4174947237049383	0.8477056404145804	0.2535205802348063
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Fe	Fe51	0.9196038473600712	0.3512136446756299	0.2555997268985414
Fe	Fe52	0.9198859488948224	0.8524609120679070	0.2564343720584347
Fe	Fe53	0.6164447629327364	0.7460767674653230	0.2809590098363243
Fe	Fe54	0.1149170431378546	0.2423195453155364	0.2804924990028814
Fe	Fe55	0.1168896782993829	0.7460828988568519	0.2809481553476477
Fe	Fe56	0.6200662667879263	0.2526928641420621	0.2780938032238180
Fe	Fe57	0.3129271419879279	0.6386959413482942	0.2994037096090616
Fe	Fe58	0.8129029780820881	0.6386197455657879	0.2992686786204798
Fe	Fe59	0.8005849851375315	0.1388662783304983	0.3009645503189137
Fe	Fe60	0.3258248443416555	0.1388438819947058	0.3009692712454080

Fe Fe61 0.5041848205310794 0.5225293986419547 0.3155097864522579

Fe Fe62 0.0071207441514672 0.0269912443436632 0.3159268944070976

Fe Fe63 0.0054533508412957 0.5224934523055492 0.3155009323550472

Fe Fe64 0.4946626536135521 0.0018434007781379 0.3162003403004204

N N65 0.5701286074194010 0.1528486164767633 0.3450750449305460

H H66 0.5836796266824972 0.1798865798895709 0.3893442530587714

6.5 NH_2 adsorption.cif

data_

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_cell_length_b 12.6651

_cell_length_c 22.0800

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

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_symmetry_space_group_name_H-M 'T'

loop_

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_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

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Fe Fe3 0.5871 0.6870 0.0000

Fe Fe4 0.0871 0.6870 0.0000

Fe Fe5 0.2815 0.5759 0.0214

Fe Fe6 0.7815 0.5759 0.0214

Fe	Fe7	0.2815	0.0759	0.0214
Fe	Fe8	0.7815	0.0759	0.0214
Fe	Fe9	0.9760	0.9648	0.0428
Fe	Fe10	0.9760	0.4648	0.0428
Fe	Fe11	0.4760	0.9648	0.0428
Fe	Fe12	0.4760	0.4648	0.0428
Fe	Fe13	0.6704	0.8537	0.0641
Fe	Fe14	0.6704	0.3537	0.0641
Fe	Fe15	0.1704	0.8537	0.0641
Fe	Fe16	0.1704	0.3537	0.0641
Fe	Fe17	0.8649	0.7426	0.0855
Fe	Fe18	0.3649	0.7426	0.0855
Fe	Fe19	0.8649	0.2426	0.0855
Fe	Fe20	0.3649	0.2426	0.0855
Fe	Fe21	0.0593	0.6315	0.1069
Fe	Fe22	0.5593	0.6315	0.1069
Fe	Fe23	0.0593	0.1315	0.1069
Fe	Fe24	0.5593	0.1315	0.1069
Fe	Fe25	0.2538	0.0204	0.1283
Fe	Fe26	0.2538	0.5204	0.1283
Fe	Fe27	0.7538	0.5204	0.1283
Fe	Fe28	0.7538	0.0204	0.1283
Fe	Fe29	0.4482	0.4092	0.1496
Fe	Fe30	0.9482	0.4092	0.1496
Fe	Fe31	0.4482	0.9093	0.1496
Fe	Fe32	0.9482	0.9093	0.1496
Fe	Fe33	0.6427	0.2981	0.1710
Fe	Fe34	0.1427	0.2981	0.1710
Fe	Fe35	0.1427	0.7981	0.1710
Fe	Fe36	0.6427	0.7981	0.1710
Fe	Fe37	0.8371	0.6870	0.1924
Fe	Fe38	0.3371	0.1870	0.1924
Fe	Fe39	0.3371	0.6870	0.1924

Fe	Fe40	0.8371	0.1870	0.1924
Fe	Fe41	0.5311806640502289	0.5757387085535828	0.2146655335475519
Fe	Fe42	0.5315802267849710	0.0761883181696675	0.2144892121431234
Fe	Fe43	0.0315322839068830	0.0760345285845393	0.2144672437678635
Fe	Fe44	0.0322014159941394	0.5764352192522056	0.2142250947904232
Fe	Fe45	0.7253132838866903	0.4634044651858483	0.2400415687624591
Fe	Fe46	0.7250299261234671	0.9630731225862935	0.2403421294180311
Fe	Fe47	0.2248674790194099	0.9631382315139160	0.2403388120700999
Fe	Fe48	0.2254111574831708	0.4634357221800257	0.2391547214136788
Fe	Fe49	0.4186758997540369	0.8511904234613874	0.2557040191832919
Fe	Fe50	0.4205409775272866	0.3532081029142050	0.2564883197425978
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Fe	Fe53	0.6160544119597008	0.7458380054577681	0.2790354503074808
Fe	Fe54	0.1159096480934371	0.2449416340433781	0.2800047640445503
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Fe	Fe57	0.3105392266282156	0.6351286670031413	0.3018814919914414
Fe	Fe58	0.8133945185196549	0.6386918857021805	0.2988274682821318
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Fe	Fe60	0.3128437328207037	0.1386703384649826	0.2992700986657494
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Fe	Fe62	0.0045108449477336	0.0220987770969876	0.3156609787702008
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6.6 NH_3 adsorption.cif

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_audit_creation_method 'generated by wxDragon 1.3.4 '

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Fe    Fe3          0.5871    0.6870    0.0000
Fe    Fe4          0.0871    0.6870    0.0000
Fe    Fe5          0.2815    0.5759    0.0214
Fe    Fe6          0.7815    0.5759    0.0214
Fe    Fe7          0.2815    0.0759    0.0214
Fe    Fe8          0.7815    0.0759    0.0214
Fe    Fe9          0.9760    0.9648    0.0428
Fe    Fe10         0.9760    0.4648    0.0428
Fe    Fe11         0.4760    0.9648    0.0428
Fe    Fe12         0.4760    0.4648    0.0428
Fe    Fe13         0.6704    0.8537    0.0641
Fe    Fe14         0.6704    0.3537    0.0641
Fe    Fe15         0.1704    0.8537    0.0641
Fe    Fe16         0.1704    0.3537    0.0641
Fe    Fe17         0.8649    0.7426    0.0855
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Fe	Fe19	0.8649	0.2426	0.0855
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Fe	Fe22	0.5593	0.6315	0.1069
Fe	Fe23	0.0593	0.1315	0.1069
Fe	Fe24	0.5593	0.1315	0.1069
Fe	Fe25	0.2538	0.0204	0.1283
Fe	Fe26	0.2538	0.5204	0.1283
Fe	Fe27	0.7538	0.5204	0.1283
Fe	Fe28	0.7538	0.0204	0.1283
Fe	Fe29	0.4482	0.4092	0.1496
Fe	Fe30	0.9482	0.4092	0.1496
Fe	Fe31	0.4482	0.9093	0.1496
Fe	Fe32	0.9482	0.9093	0.1496
Fe	Fe33	0.6427	0.2981	0.1710
Fe	Fe34	0.1427	0.2981	0.1710
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Fe	Fe36	0.6427	0.7981	0.1710
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Fe	Fe38	0.3371	0.1870	0.1924
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6.7 N_2 activation.cif

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Fe	Fe6	0.7815	0.5759	0.0214
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Fe	Fe30	0.9482	0.4092	0.1496
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Fe	Fe32	0.9482	0.9093	0.1496
Fe	Fe33	0.6427	0.2981	0.1710
Fe	Fe34	0.1427	0.2981	0.1710
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Fe	Fe36	0.6427	0.7981	0.1710
Fe	Fe37	0.8371	0.6870	0.1924
Fe	Fe38	0.3371	0.1870	0.1924
Fe	Fe39	0.3371	0.6870	0.1924
Fe	Fe40	0.8371	0.1870	0.1924
Fe	Fe41	0.5301	0.5764	0.2150
Fe	Fe42	0.5325	0.0771	0.2150
Fe	Fe43	0.0319	0.0754	0.2144
Fe	Fe44	0.0334	0.5764	0.2150
Fe	Fe45	0.7231	0.4625	0.2375
Fe	Fe46	0.7257	0.9625	0.2401
Fe	Fe47	0.2257	0.9630	0.2407
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Fe	Fe52	0.9191	0.8503	0.2561
Fe	Fe53	0.6159	0.7459	0.2806
Fe	Fe54	0.1164	0.2427	0.2795
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6.8 N+H hydrogenation.cif

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_cell_length_c 22.0800

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 108.4350

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

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Fe Fe3 0.5871 0.6870 0.0000

Fe Fe4 0.0871 0.6870 0.0000

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Fe Fe6 0.7815 0.5759 0.0214

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Fe	Fe8	0.7815	0.0759	0.0214
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Fe	Fe11	0.4760	0.9648	0.0428
Fe	Fe12	0.4760	0.4648	0.0428
Fe	Fe13	0.6704	0.8537	0.0641
Fe	Fe14	0.6704	0.3537	0.0641
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Fe	Fe16	0.1704	0.3537	0.0641
Fe	Fe17	0.8649	0.7426	0.0855
Fe	Fe18	0.3649	0.7426	0.0855
Fe	Fe19	0.8649	0.2426	0.0855
Fe	Fe20	0.3649	0.2426	0.0855
Fe	Fe21	0.0593	0.6315	0.1069
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Fe	Fe23	0.0593	0.1315	0.1069
Fe	Fe24	0.5593	0.1315	0.1069
Fe	Fe25	0.2538	0.0204	0.1283
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Fe	Fe32	0.9482	0.9093	0.1496
Fe	Fe33	0.6427	0.2981	0.1710
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6.9 HN+H hydrogenation.cif

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_cell_angle_gamma 108.4350

_symmetry_space_group_name_H-M 'T'

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_atom_site_label

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Fe	Fe4	0.0871	0.6870	0.0000
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Fe	Fe6	0.7815	0.5759	0.0214
Fe	Fe7	0.2815	0.0759	0.0214
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Fe	Fe29	0.4482	0.4092	0.1496
Fe	Fe30	0.9482	0.4092	0.1496
Fe	Fe31	0.4482	0.9093	0.1496
Fe	Fe32	0.9482	0.9093	0.1496
Fe	Fe33	0.6427	0.2981	0.1710
Fe	Fe34	0.1427	0.2981	0.1710
Fe	Fe35	0.1427	0.7981	0.1710
Fe	Fe36	0.6427	0.7981	0.1710
Fe	Fe37	0.8371	0.6870	0.1924
Fe	Fe38	0.3371	0.1870	0.1924
Fe	Fe39	0.3371	0.6870	0.1924
Fe	Fe40	0.8371	0.1870	0.1924
Fe	Fe41	0.5309933560278716	0.5746912270835457	0.2143533669575487
Fe	Fe42	0.5314376882546742	0.0764853365961794	0.2145243227379664
Fe	Fe43	0.0315564593796797	0.0762235390623789	0.2146867360628615
Fe	Fe44	0.0320953874179846	0.5761822484491516	0.2146956744491539
Fe	Fe45	0.7255210776560136	0.4625487021410575	0.2406366770157709
Fe	Fe46	0.7252453074712375	0.9639707516978306	0.2402881399306636
Fe	Fe47	0.2240505063036755	0.9632429889413805	0.2406065179209013
Fe	Fe48	0.2247226120158513	0.4627028728622464	0.2409841884258669
Fe	Fe49	0.4191170223443116	0.8518046929698059	0.2554210329597687
Fe	Fe50	0.4182732069520727	0.3492658394419580	0.2543739791645047
Fe	Fe51	0.9191466714809079	0.3513478926334505	0.2557340494195280

Fe	Fe52	0.9179069182377038	0.8514631223983692	0.2571781366229755
Fe	Fe53	0.6153213640854301	0.7481167532777674	0.2790934054990535
Fe	Fe54	0.1163472505699244	0.2457577820830518	0.2809893920435638
Fe	Fe55	0.1171751654609445	0.7444686312597687	0.2790608776708314
Fe	Fe56	0.6158882583296490	0.2463506119988751	0.2810644303786486
Fe	Fe57	0.3152657078298526	0.6385352596304386	0.3002424893509980
Fe	Fe58	0.8129913256777578	0.6381243773141692	0.2996168045077598
Fe	Fe59	0.8120311875774171	0.1387777944957274	0.2993234209929113
Fe	Fe60	0.3128948626604257	0.1390977250874590	0.2994371224629768
Fe	Fe61	0.4985140678829037	0.5078972545475099	0.3161792962917874
Fe	Fe62	0.0059750065936697	0.0247080317118293	0.3161333135413327
Fe	Fe63	1.0029246027035967	0.5215473213522465	0.3156696801048943
Fe	Fe64	0.5036762324104218	0.0231101389528337	0.3155519952796455
N	N65	0.5237369519837958	0.6521916173728352	0.3533046737771464
H	H66	0.6966444374023796	0.7216628356622841	0.3457642513497076
H	H67	0.5185582287834968	0.6720976956302519	0.3982760049909538

6.10 H_2N+H hydrogenation.cif

data_

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_cell_length_a 8.0101
_cell_length_b 12.6651
_cell_length_c 22.0800
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 108.4350

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.5871	0.1870	0.0000
Fe	Fe2	0.0871	0.1870	0.0000
Fe	Fe3	0.5871	0.6870	0.0000
Fe	Fe4	0.0871	0.6870	0.0000
Fe	Fe5	0.2815	0.5759	0.0214
Fe	Fe6	0.7815	0.5759	0.0214
Fe	Fe7	0.2815	0.0759	0.0214
Fe	Fe8	0.7815	0.0759	0.0214
Fe	Fe9	0.9760	0.9648	0.0428
Fe	Fe10	0.9760	0.4648	0.0428
Fe	Fe11	0.4760	0.9648	0.0428
Fe	Fe12	0.4760	0.4648	0.0428
Fe	Fe13	0.6704	0.8537	0.0641
Fe	Fe14	0.6704	0.3537	0.0641
Fe	Fe15	0.1704	0.8537	0.0641
Fe	Fe16	0.1704	0.3537	0.0641
Fe	Fe17	0.8649	0.7426	0.0855
Fe	Fe18	0.3649	0.7426	0.0855
Fe	Fe19	0.8649	0.2426	0.0855
Fe	Fe20	0.3649	0.2426	0.0855
Fe	Fe21	0.0593	0.6315	0.1069
Fe	Fe22	0.5593	0.6315	0.1069
Fe	Fe23	0.0593	0.1315	0.1069
Fe	Fe24	0.5593	0.1315	0.1069
Fe	Fe25	0.2538	0.0204	0.1283
Fe	Fe26	0.2538	0.5204	0.1283
Fe	Fe27	0.7538	0.5204	0.1283
Fe	Fe28	0.7538	0.0204	0.1283
Fe	Fe29	0.4482	0.4092	0.1496

Fe	Fe30	0.9482	0.4092	0.1496
Fe	Fe31	0.4482	0.9093	0.1496
Fe	Fe32	0.9482	0.9093	0.1496
Fe	Fe33	0.6427	0.2981	0.1710
Fe	Fe34	0.1427	0.2981	0.1710
Fe	Fe35	0.1427	0.7981	0.1710
Fe	Fe36	0.6427	0.7981	0.1710
Fe	Fe37	0.8371	0.6870	0.1924
Fe	Fe38	0.3371	0.1870	0.1924
Fe	Fe39	0.3371	0.6870	0.1924
Fe	Fe40	0.8371	0.1870	0.1924
Fe	Fe41	0.5311486423174258	0.5757507966750366	0.2147721370479057
Fe	Fe42	0.5314348800337546	0.0760520622550007	0.2143252485929442
Fe	Fe43	0.0316058830538461	0.0761320258217631	0.2144458075541228
Fe	Fe44	0.0316577580231654	0.5763692065146629	0.2145664162095123
Fe	Fe45	0.7251783574062607	0.4625256440433165	0.2388875203304977
Fe	Fe46	0.7256009154412467	0.9632496045108186	0.2403708985352200
Fe	Fe47	0.2245312270516053	0.9629834653803961	0.2404679721604565
Fe	Fe48	0.2250710405137360	0.4632203515370084	0.2401152056474106
Fe	Fe49	0.4192385815934380	0.8517564740025394	0.2557385858700599
Fe	Fe50	0.4195746933264196	0.3531610347267095	0.2564186502815951
Fe	Fe51	0.9191888045621780	0.3520970646905677	0.2559369978094236
Fe	Fe52	0.9191181559867231	0.8502249755418387	0.2561793470954737
Fe	Fe53	0.6171390438545729	0.7458838869581806	0.2790856904158842
Fe	Fe54	0.1162308200307042	0.2461338368738096	0.2805831861065552
Fe	Fe55	0.1141559354370039	0.7452008546149008	0.2807041238992774
Fe	Fe56	0.6158427623809566	0.2449834479418845	0.2798581163144086
Fe	Fe57	0.3148792717379705	0.6396496839817464	0.2987306442936111
Fe	Fe58	0.8098506655121026	0.6320560333613533	0.2997074091812463
Fe	Fe59	0.8130982946361620	0.1389354143142019	0.2993497559831618
Fe	Fe60	0.3125946603513394	0.1387471406103373	0.2992728948385418
Fe	Fe61	0.5006361883951063	0.5244713587561721	0.3182795627956632
Fe	Fe62	0.0044185074336987	0.0227301859621096	0.3154026638640299

Fe Fe63 0.0140780869974178 0.5227462497382995 0.3159975710557437

Fe Fe64 0.5049891830334670 0.0228360559637750 0.3153962985785099

N N65 0.6803409915607269 0.5550697410238336 0.3853866639155428

H H66 0.8545394228191420 0.5790992717454249 0.3657599386492037

H H67 0.6820674468616349 0.6122050168837752 0.4185277799860794

H H68 0.6804494437281212 0.4820972728419209 0.4056751619199381

7. (310) surface

7.1 H adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 5.6640

_cell_length_b 9.3927

_cell_length_c 24.8511

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 72.4516

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe Fe1 0.8084 0.2915 0.0000

Fe Fe2 0.3085 0.2915 0.0000

Fe Fe3 0.3085 0.7915 0.0000

Fe Fe4 0.8084 0.7915 0.0000

Fe	Fe5	0.9585	0.9915	0.0360
Fe	Fe6	0.4584	0.9915	0.0360
Fe	Fe7	0.9585	0.4915	0.0360
Fe	Fe8	0.4584	0.4915	0.0360
Fe	Fe9	0.1085	0.6915	0.0721
Fe	Fe10	0.6084	0.6915	0.0721
Fe	Fe11	0.1085	0.1915	0.0721
Fe	Fe12	0.6084	0.1915	0.0721
Fe	Fe13	0.2585	0.8915	0.1081
Fe	Fe14	0.7584	0.8915	0.1081
Fe	Fe15	0.2585	0.3915	0.1081
Fe	Fe16	0.7584	0.3915	0.1081
Fe	Fe17	0.9085	0.0915	0.1442
Fe	Fe18	0.4085	0.0915	0.1442
Fe	Fe19	0.4085	0.5915	0.1442
Fe	Fe20	0.9085	0.5915	0.1442
Fe	Fe21	0.5584	0.2915	0.1802
Fe	Fe22	0.0584	0.2915	0.1802
Fe	Fe23	0.5584	0.7915	0.1802
Fe	Fe24	0.0584	0.7915	0.1802
Fe	Fe25	0.2085	0.9915	0.2162
Fe	Fe26	0.7085	0.9915	0.2162
Fe	Fe27	0.7085	0.4915	0.2162
Fe	Fe28	0.2085	0.4915	0.2162
Fe	Fe29	0.3584	0.1915	0.2523
Fe	Fe30	0.8584	0.6915	0.2523
Fe	Fe31	0.8584	0.1915	0.2523
Fe	Fe32	0.3584	0.6915	0.2523
Fe	Fe33	0.0089413275134792	0.8903801530903223	0.2889320610358894
Fe	Fe34	0.0088079189445182	0.3900976780706596	0.2890337425330891
Fe	Fe35	0.5093168610817737	0.3901270722458918	0.2890286520465011
Fe	Fe36	0.5088704576980324	0.8905744634008479	0.2889824354913371
Fe	Fe37	0.6583676876372448	0.0933403373080807	0.3246752083337630

Fe	Fe38	0.1563293312881846	0.0933541282749194	0.3246743443675270
Fe	Fe39	0.6574596024546544	0.5931800108916078	0.3244510456679750
Fe	Fe40	0.1578603998711184	0.5923018094008778	0.3247344888843927
Fe	Fe41	0.3067496319627781	0.7920386229278684	0.3633195489227451
Fe	Fe42	0.8092561884963485	0.7920198719886041	0.3633399686383266
Fe	Fe43	0.8068605103885654	0.2943234285298061	0.3648173586545461
Fe	Fe44	0.3072736597820951	0.2935318314230514	0.3633497240502850
Fe	Fe45	0.9554088778258281	0.5017263019898328	0.3953010140914672
Fe	Fe46	0.4508274964792795	0.5017729406428385	0.3952790179846584
Fe	Fe47	0.4533431559763166	0.0012008249657804	0.3940033432656349
Fe	Fe48	0.9531213164734207	0.0016297384651914	0.3945897743640108
H	H49	0.7496180409314501	0.4086827677132302	0.4241250283094559

7.2 N adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 5.6640
_cell_length_b 9.3927
_cell_length_c 24.8511
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 72.4516

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

Fe	Fe1	0.8084	0.2915	0.0000
Fe	Fe2	0.3085	0.2915	0.0000
Fe	Fe3	0.3085	0.7915	0.0000
Fe	Fe4	0.8084	0.7915	0.0000
Fe	Fe5	0.9585	0.9915	0.0360
Fe	Fe6	0.4584	0.9915	0.0360
Fe	Fe7	0.9585	0.4915	0.0360
Fe	Fe8	0.4584	0.4915	0.0360
Fe	Fe9	0.1085	0.6915	0.0721
Fe	Fe10	0.6084	0.6915	0.0721
Fe	Fe11	0.1085	0.1915	0.0721
Fe	Fe12	0.6084	0.1915	0.0721
Fe	Fe13	0.2585	0.8915	0.1081
Fe	Fe14	0.7584	0.8915	0.1081
Fe	Fe15	0.2585	0.3915	0.1081
Fe	Fe16	0.7584	0.3915	0.1081
Fe	Fe17	0.9085	0.0915	0.1442
Fe	Fe18	0.4085	0.0915	0.1442
Fe	Fe19	0.4085	0.5915	0.1442
Fe	Fe20	0.9085	0.5915	0.1442
Fe	Fe21	0.5584	0.2915	0.1802
Fe	Fe22	0.0584	0.2915	0.1802
Fe	Fe23	0.5584	0.7915	0.1802
Fe	Fe24	0.0584	0.7915	0.1802
Fe	Fe25	0.2085	0.9915	0.2162
Fe	Fe26	0.7085	0.9915	0.2162
Fe	Fe27	0.7085	0.4915	0.2162
Fe	Fe28	0.2085	0.4915	0.2162
Fe	Fe29	0.3584	0.1915	0.2523
Fe	Fe30	0.8584	0.6915	0.2523
Fe	Fe31	0.8584	0.1915	0.2523
Fe	Fe32	0.3584	0.6915	0.2523
Fe	Fe33	0.0100	0.8882	0.2902

Fe	Fe34	0.0103	0.3892	0.2891
Fe	Fe35	0.5087	0.3892	0.2891
Fe	Fe36	0.5086	0.8910	0.2890
Fe	Fe37	0.6584	0.0932	0.3248
Fe	Fe38	0.1563	0.0932	0.3248
Fe	Fe39	0.6602	0.5877	0.3203
Fe	Fe40	0.1578	0.5925	0.3249
Fe	Fe41	0.3190	0.7901	0.3647
Fe	Fe42	0.7988	0.7902	0.3647
Fe	Fe43	0.8086	0.2909	0.3644
Fe	Fe44	0.3051	0.2975	0.3634
Fe	Fe45	0.9482	0.5040	0.3951
Fe	Fe46	0.4557	0.5039	0.3951
Fe	Fe47	0.4487	0.0103	0.3942
Fe	Fe48	0.9557	0.9967	0.3944
N	N49	0.6268	0.6541	0.3940

7.3 N_2 adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

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_cell_length_b 9.3927
_cell_length_c 24.8511
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 72.4516

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.3085	0.2915	0.0000
Fe	Fe3	0.3085	0.7915	0.0000
Fe	Fe4	0.8084	0.7915	0.0000
Fe	Fe5	0.9585	0.9915	0.0360
Fe	Fe6	0.4584	0.9915	0.0360
Fe	Fe7	0.9585	0.4915	0.0360
Fe	Fe8	0.4584	0.4915	0.0360
Fe	Fe9	0.1085	0.6915	0.0721
Fe	Fe10	0.6084	0.6915	0.0721
Fe	Fe11	0.1085	0.1915	0.0721
Fe	Fe12	0.6084	0.1915	0.0721
Fe	Fe13	0.2585	0.8915	0.1081
Fe	Fe14	0.7584	0.8915	0.1081
Fe	Fe15	0.2585	0.3915	0.1081
Fe	Fe16	0.7584	0.3915	0.1081
Fe	Fe17	0.9085	0.0915	0.1442
Fe	Fe18	0.4085	0.0915	0.1442
Fe	Fe19	0.4085	0.5915	0.1442
Fe	Fe20	0.9085	0.5915	0.1442
Fe	Fe21	0.5584	0.2915	0.1802
Fe	Fe22	0.0584	0.2915	0.1802
Fe	Fe23	0.5584	0.7915	0.1802
Fe	Fe24	0.0584	0.7915	0.1802
Fe	Fe25	0.2085	0.9915	0.2162
Fe	Fe26	0.7085	0.9915	0.2162
Fe	Fe27	0.7085	0.4915	0.2162
Fe	Fe28	0.2085	0.4915	0.2162
Fe	Fe29	0.3584	0.1915	0.2523

Fe	Fe30	0.8584	0.6915	0.2523
Fe	Fe31	0.8584	0.1915	0.2523
Fe	Fe32	0.3584	0.6915	0.2523
Fe	Fe33	0.0090260954505618	0.8901981990183614	0.2894158759563195
Fe	Fe34	0.0099938013309699	0.3896487126750862	0.2891693946310379
Fe	Fe35	0.5085394789154126	0.3896500633697066	0.2891614047932654
Fe	Fe36	0.5086851244705788	0.8908698962200915	0.2888485077176635
Fe	Fe37	0.6541513862396262	0.0938889008567190	0.3248443837727929
Fe	Fe38	0.1600243387780732	0.0938731893621943	0.3248606071810366
Fe	Fe39	0.6590077827990626	0.5899641801263563	0.3236661520988827
Fe	Fe40	0.1585517392955001	0.5908675096154681	0.3249356840645753
Fe	Fe41	0.2972152439349857	0.7967971047097056	0.3631513220463585
Fe	Fe42	0.8140015428093131	0.7967645695002057	0.3631601084144866
Fe	Fe43	0.8076716986693621	0.2926839728130655	0.3641172421575583
Fe	Fe44	0.3070062714033668	0.2939479758493992	0.3641937722202271
Fe	Fe45	0.9604960863469696	0.4991133604757335	0.3968748591428126
Fe	Fe46	0.4483956640370599	0.4991632346398944	0.3968513363542341
Fe	Fe47	0.4559852843779249	0.9965619158097241	0.3969195803264672
Fe	Fe48	0.9484488859675005	0.0108259318226185	0.3936512375968833
N	N49	0.6325335320923050	0.6428314109826205	0.4107464243152776
N	N50	0.5606153398306519	0.7860234951977521	0.4201871067477831

7.4 NH adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 5.6640

_cell_length_b 9.3927

_cell_length_c 24.8511

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 72.4516

_symmetry_space_group_name_H-M 'T'

loop_

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_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.3085	0.2915	0.0000
Fe	Fe3	0.3085	0.7915	0.0000
Fe	Fe4	0.8084	0.7915	0.0000
Fe	Fe5	0.9585	0.9915	0.0360
Fe	Fe6	0.4584	0.9915	0.0360
Fe	Fe7	0.9585	0.4915	0.0360
Fe	Fe8	0.4584	0.4915	0.0360
Fe	Fe9	0.1085	0.6915	0.0721
Fe	Fe10	0.6084	0.6915	0.0721
Fe	Fe11	0.1085	0.1915	0.0721
Fe	Fe12	0.6084	0.1915	0.0721
Fe	Fe13	0.2585	0.8915	0.1081
Fe	Fe14	0.7584	0.8915	0.1081
Fe	Fe15	0.2585	0.3915	0.1081
Fe	Fe16	0.7584	0.3915	0.1081
Fe	Fe17	0.9085	0.0915	0.1442
Fe	Fe18	0.4085	0.0915	0.1442
Fe	Fe19	0.4085	0.5915	0.1442
Fe	Fe20	0.9085	0.5915	0.1442
Fe	Fe21	0.5584	0.2915	0.1802
Fe	Fe22	0.0584	0.2915	0.1802
Fe	Fe23	0.5584	0.7915	0.1802
Fe	Fe24	0.0584	0.7915	0.1802

Fe	Fe25	0.2085	0.9915	0.2162
Fe	Fe26	0.7085	0.9915	0.2162
Fe	Fe27	0.7085	0.4915	0.2162
Fe	Fe28	0.2085	0.4915	0.2162
Fe	Fe29	0.3584	0.1915	0.2523
Fe	Fe30	0.8584	0.6915	0.2523
Fe	Fe31	0.8584	0.1915	0.2523
Fe	Fe32	0.3584	0.6915	0.2523
Fe	Fe33	0.0088484094881898	0.8904464244645069	0.2887442558956286
Fe	Fe34	0.0087267819872839	0.3900220832693994	0.2893032050771367
Fe	Fe35	0.5094095017246690	0.3900225638314756	0.2893183761050451
Fe	Fe36	0.5086205708366027	0.8909496605604298	0.2885414868168514
Fe	Fe37	0.6582831481681974	0.0923603700569815	0.3247547367938102
Fe	Fe38	0.1574558781734792	0.0923365113532672	0.3247466870973082
Fe	Fe39	0.6576577517506279	0.5926300222327968	0.3241145738760329
Fe	Fe40	0.1578449280928416	0.5921206009930531	0.3236258140787968
Fe	Fe41	0.3078318171970039	0.7900873050327408	0.3626933712359721
Fe	Fe42	0.8101266827226149	0.7901043880341264	0.3627082359816583
Fe	Fe43	0.8089694899744625	0.2901756148235926	0.3656715480123772
Fe	Fe44	0.3065055327794709	0.2948908654605035	0.3622570168533997
Fe	Fe45	0.9656484738278491	0.5049692119215577	0.3967408299570764
Fe	Fe46	0.4367343468404373	0.5051766957965292	0.3967328293995483
Fe	Fe47	0.4553716674284501	0.9972909631340977	0.3938418355078392
Fe	Fe48	0.9544982332720299	-0.0008740661191049	0.3943690233423324
N	N49	0.7473726869237476	0.4124767720085836	0.4298380895144117
H	H50	0.7698675700224421	0.3671471085646867	0.4678838650608901

7.5 NH_2 adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

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_cell_length_b 9.3927

_cell_length_c 24.8511

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 72.4516

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.8084	0.2915	0.0000
Fe	Fe2	0.3085	0.2915	0.0000
Fe	Fe3	0.3085	0.7915	0.0000
Fe	Fe4	0.8084	0.7915	0.0000
Fe	Fe5	0.9585	0.9915	0.0360
Fe	Fe6	0.4584	0.9915	0.0360
Fe	Fe7	0.9585	0.4915	0.0360
Fe	Fe8	0.4584	0.4915	0.0360
Fe	Fe9	0.1085	0.6915	0.0721
Fe	Fe10	0.6084	0.6915	0.0721
Fe	Fe11	0.1085	0.1915	0.0721
Fe	Fe12	0.6084	0.1915	0.0721
Fe	Fe13	0.2585	0.8915	0.1081
Fe	Fe14	0.7584	0.8915	0.1081
Fe	Fe15	0.2585	0.3915	0.1081
Fe	Fe16	0.7584	0.3915	0.1081
Fe	Fe17	0.9085	0.0915	0.1442
Fe	Fe18	0.4085	0.0915	0.1442
Fe	Fe19	0.4085	0.5915	0.1442

Fe	Fe20	0.9085	0.5915	0.1442
Fe	Fe21	0.5584	0.2915	0.1802
Fe	Fe22	0.0584	0.2915	0.1802
Fe	Fe23	0.5584	0.7915	0.1802
Fe	Fe24	0.0584	0.7915	0.1802
Fe	Fe25	0.2085	0.9915	0.2162
Fe	Fe26	0.7085	0.9915	0.2162
Fe	Fe27	0.7085	0.4915	0.2162
Fe	Fe28	0.2085	0.4915	0.2162
Fe	Fe29	0.3584	0.1915	0.2523
Fe	Fe30	0.8584	0.6915	0.2523
Fe	Fe31	0.8584	0.1915	0.2523
Fe	Fe32	0.3584	0.6915	0.2523
Fe	Fe33	0.0087340662228761	0.8905832894584234	0.2885997298261346
Fe	Fe34	0.0097279732325393	0.3907163990185597	0.2892299762645253
Fe	Fe35	0.5075524193568725	0.3907046720901847	0.2892255425917203
Fe	Fe36	0.5087295455067282	0.8906042775149351	0.2886997826184372
Fe	Fe37	0.6567225237755063	0.0924409325148277	0.3244136140613008
Fe	Fe38	0.1586260348834451	0.0924452566331608	0.3244131592469023
Fe	Fe39	0.6577433410941000	0.5921137297585521	0.3243981605906101
Fe	Fe40	0.1582590322296627	0.5909338497791679	0.3252789597685408
Fe	Fe41	0.3057176857694813	0.7922430070791162	0.3622295428707253
Fe	Fe42	0.8098099700013560	0.7921854310470985	0.3622468204978039
Fe	Fe43	0.8083660360667000	0.2908168399130616	0.3618735246825779
Fe	Fe44	0.3060939761446637	0.2949693285741962	0.3640505403469598
Fe	Fe45	0.9453715717084444	0.5019042092047001	0.3977132630838111
Fe	Fe46	0.4594295500563248	0.5017380287100375	0.3975963123713574
Fe	Fe47	0.4535657627045070	0.0006300637225933	0.3939195455300593
Fe	Fe48	0.9535446362332660	0.0006859411693441	0.3940036665391084
N	N49	0.7000638958903126	0.5054890050059697	0.4559756345248915
H	H50	0.7440523104952235	0.4168759448057482	0.4820581757855479
H	H51	0.6511407850426101	0.6022839287158849	0.4781145212724073

7.6 NH_3 adsorption.cif

data_

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_cell_length_c 24.8511
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 72.4516

_symmetry_space_group_name_H-M 'T'

loop_
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_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

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Fe	Fe3	0.3085	0.7915	0.0000
Fe	Fe4	0.8084	0.7915	0.0000
Fe	Fe5	0.9585	0.9915	0.0360
Fe	Fe6	0.4584	0.9915	0.0360
Fe	Fe7	0.9585	0.4915	0.0360
Fe	Fe8	0.4584	0.4915	0.0360
Fe	Fe9	0.1085	0.6915	0.0721
Fe	Fe10	0.6084	0.6915	0.0721
Fe	Fe11	0.1085	0.1915	0.0721
Fe	Fe12	0.6084	0.1915	0.0721
Fe	Fe13	0.2585	0.8915	0.1081

Fe	Fe14	0.7584	0.8915	0.1081
Fe	Fe15	0.2585	0.3915	0.1081
Fe	Fe16	0.7584	0.3915	0.1081
Fe	Fe17	0.9085	0.0915	0.1442
Fe	Fe18	0.4085	0.0915	0.1442
Fe	Fe19	0.4085	0.5915	0.1442
Fe	Fe20	0.9085	0.5915	0.1442
Fe	Fe21	0.5584	0.2915	0.1802
Fe	Fe22	0.0584	0.2915	0.1802
Fe	Fe23	0.5584	0.7915	0.1802
Fe	Fe24	0.0584	0.7915	0.1802
Fe	Fe25	0.2085	0.9915	0.2162
Fe	Fe26	0.7085	0.9915	0.2162
Fe	Fe27	0.7085	0.4915	0.2162
Fe	Fe28	0.2085	0.4915	0.2162
Fe	Fe29	0.3584	0.1915	0.2523
Fe	Fe30	0.8584	0.6915	0.2523
Fe	Fe31	0.8584	0.1915	0.2523
Fe	Fe32	0.3584	0.6915	0.2523
Fe	Fe33	0.0087263810388674	0.8903989379256004	0.2889171135157631
Fe	Fe34	0.0088531016926258	0.3905100359236064	0.2890060100847082
Fe	Fe35	0.5089272383874370	0.3902657133358284	0.2893304761112568
Fe	Fe36	0.5091003201867964	0.8904199713633542	0.2889194595294195
Fe	Fe37	0.6576696828790021	0.0925548325818053	0.3248065931117425
Fe	Fe38	0.1575526177561041	0.0928827118701366	0.3247693832157594
Fe	Fe39	0.6550765201376546	0.5927466659990845	0.3244641180661617
Fe	Fe40	0.1601181271632242	0.5927233855785027	0.3245576490534253
Fe	Fe41	0.3067738171305748	0.7943463895717652	0.3632169432627163
Fe	Fe42	0.8074773659114659	0.7928893297428484	0.3635790066408557
Fe	Fe43	0.8056637732668956	0.2931672786913740	0.3636102324572519
Fe	Fe44	0.3090050085382477	0.2932853377650017	0.3636077022026755
Fe	Fe45	0.9523347995676169	0.5019025520418448	0.3925685460450545
Fe	Fe46	0.4529871831740083	0.5025982384509193	0.3977315417410475

Fe Fe47 0.4536812470173547 0.0012405314039540 0.3947006687462314

Fe Fe48 0.9527692336062855 0.0011913670859545 0.3947042698478588

N N49 0.4186806632180423 0.5476602352140935 0.4820329866970241

H H50 0.4161535187972088 0.4564424143020049 0.5043844102464451

H H51 0.2551864962052779 0.6310570995172727 0.4877928617963864

H H52 0.5591783403931162 0.5860602130476281 0.4956595711142481

7.7 N_2 activation.cif

data_

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_cell_length_a 5.6640

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_cell_length_c 24.8511

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 72.4516

_symmetry_space_group_name_H-M 'T'

loop_

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_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

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Fe Fe3 0.3085 0.7915 0.0000

Fe Fe4 0.8084 0.7915 0.0000

Fe Fe5 0.9585 0.9915 0.0360

Fe Fe6 0.4584 0.9915 0.0360

Fe	Fe7	0.9585	0.4915	0.0360
Fe	Fe8	0.4584	0.4915	0.0360
Fe	Fe9	0.1085	0.6915	0.0721
Fe	Fe10	0.6084	0.6915	0.0721
Fe	Fe11	0.1085	0.1915	0.0721
Fe	Fe12	0.6084	0.1915	0.0721
Fe	Fe13	0.2585	0.8915	0.1081
Fe	Fe14	0.7584	0.8915	0.1081
Fe	Fe15	0.2585	0.3915	0.1081
Fe	Fe16	0.7584	0.3915	0.1081
Fe	Fe17	0.9085	0.0915	0.1442
Fe	Fe18	0.4085	0.0915	0.1442
Fe	Fe19	0.4085	0.5915	0.1442
Fe	Fe20	0.9085	0.5915	0.1442
Fe	Fe21	0.5584	0.2915	0.1802
Fe	Fe22	0.0584	0.2915	0.1802
Fe	Fe23	0.5584	0.7915	0.1802
Fe	Fe24	0.0584	0.7915	0.1802
Fe	Fe25	0.2085	0.9915	0.2162
Fe	Fe26	0.7085	0.9915	0.2162
Fe	Fe27	0.7085	0.4915	0.2162
Fe	Fe28	0.2085	0.4915	0.2162
Fe	Fe29	0.3584	0.1915	0.2523
Fe	Fe30	0.8584	0.6915	0.2523
Fe	Fe31	0.8584	0.1915	0.2523
Fe	Fe32	0.3584	0.6915	0.2523
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Fe	Fe36	0.5088	0.8906	0.2891
Fe	Fe37	0.6570	0.0925	0.3241
Fe	Fe38	0.1584	0.0925	0.3241
Fe	Fe39	0.6594	0.5896	0.3225

Fe Fe40 0.1586 0.5910 0.3252

Fe Fe41 0.3083 0.7953 0.3650

Fe Fe42 0.8039 0.7951 0.3651

Fe Fe43 0.8095 0.2897 0.3641

Fe Fe44 0.3082 0.2924 0.3629

Fe Fe45 0.9611 0.4959 0.3960

Fe Fe46 0.4519 0.4961 0.3959

Fe Fe47 0.4422 0.0233 0.3987

Fe Fe48 0.9513 0.0047 0.3931

N N49 0.6369 0.6356 0.3998

N N50 0.5418 0.8232 0.4153

7.8 N+H hydrogenation.cif

data_

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_cell_length_c 24.8511

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 72.4516

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe4	0.8084	0.7915	0.0000
Fe	Fe5	0.9585	0.9915	0.0360
Fe	Fe6	0.4584	0.9915	0.0360
Fe	Fe7	0.9585	0.4915	0.0360
Fe	Fe8	0.4584	0.4915	0.0360
Fe	Fe9	0.1085	0.6915	0.0721
Fe	Fe10	0.6084	0.6915	0.0721
Fe	Fe11	0.1085	0.1915	0.0721
Fe	Fe12	0.6084	0.1915	0.0721
Fe	Fe13	0.2585	0.8915	0.1081
Fe	Fe14	0.7584	0.8915	0.1081
Fe	Fe15	0.2585	0.3915	0.1081
Fe	Fe16	0.7584	0.3915	0.1081
Fe	Fe17	0.9085	0.0915	0.1442
Fe	Fe18	0.4085	0.0915	0.1442
Fe	Fe19	0.4085	0.5915	0.1442
Fe	Fe20	0.9085	0.5915	0.1442
Fe	Fe21	0.5584	0.2915	0.1802
Fe	Fe22	0.0584	0.2915	0.1802
Fe	Fe23	0.5584	0.7915	0.1802
Fe	Fe24	0.0584	0.7915	0.1802
Fe	Fe25	0.2085	0.9915	0.2162
Fe	Fe26	0.7085	0.9915	0.2162
Fe	Fe27	0.7085	0.4915	0.2162
Fe	Fe28	0.2085	0.4915	0.2162
Fe	Fe29	0.3584	0.1915	0.2523
Fe	Fe30	0.8584	0.6915	0.2523
Fe	Fe31	0.8584	0.1915	0.2523
Fe	Fe32	0.3584	0.6915	0.2523
Fe	Fe33	0.0094854404567837	0.8892197187199339	0.2898624415928580
Fe	Fe34	0.0099829422012497	0.3893299242985470	0.2890363626756142

Fe	Fe35	0.5089060254878228	0.3893341192783039	0.2890425871378636
Fe	Fe36	0.5084395129443300	0.8914016219141042	0.2889146178559608
Fe	Fe37	0.6589635279958101	0.0934823129049208	0.3247682780542859
Fe	Fe38	0.1556673329201510	0.0934605909864832	0.3247524150075798
Fe	Fe39	0.6591067753163975	0.5898775840507708	0.3218412268424182
Fe	Fe40	0.1585583751595525	0.5908963592780669	0.3247677938856232
Fe	Fe41	0.3070953320708817	0.7925636079084604	0.3641363387709733
Fe	Fe42	0.8083766172574721	0.7925736403674523	0.3641500302061630
Fe	Fe43	0.8086125251288061	0.2910091410712127	0.3644053729050737
Fe	Fe44	0.3061339100085814	0.2956371996889894	0.3633701719921518
Fe	Fe45	0.9547094982138836	0.5010648166705574	0.3954483604554052
Fe	Fe46	0.4522687193603351	0.5010525794005758	0.3954086553507889
Fe	Fe47	0.4501285018891368	1.0075766804923680	0.3940421979784107
Fe	Fe48	0.9540474268466446	1.0000507094727167	0.3954742538222820
N	N49	0.6303078466521896	0.6472892082411867	0.3982604599970467
H	H50	0.5568010336245309	0.7942127270965935	0.4127092454395238

7.9 HN+H hydrogenation.cif

data_

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_cell_length_c 24.8511
_cell_angle_alpha 90.0000
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_cell_angle_gamma 72.4516

_symmetry_space_group_name_H-M 'T'

loop_
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Fe	Fe3	0.3085	0.7915	0.0000
Fe	Fe4	0.8084	0.7915	0.0000
Fe	Fe5	0.9585	0.9915	0.0360
Fe	Fe6	0.4584	0.9915	0.0360
Fe	Fe7	0.9585	0.4915	0.0360
Fe	Fe8	0.4584	0.4915	0.0360
Fe	Fe9	0.1085	0.6915	0.0721
Fe	Fe10	0.6084	0.6915	0.0721
Fe	Fe11	0.1085	0.1915	0.0721
Fe	Fe12	0.6084	0.1915	0.0721
Fe	Fe13	0.2585	0.8915	0.1081
Fe	Fe14	0.7584	0.8915	0.1081
Fe	Fe15	0.2585	0.3915	0.1081
Fe	Fe16	0.7584	0.3915	0.1081
Fe	Fe17	0.9085	0.0915	0.1442
Fe	Fe18	0.4085	0.0915	0.1442
Fe	Fe19	0.4085	0.5915	0.1442
Fe	Fe20	0.9085	0.5915	0.1442
Fe	Fe21	0.5584	0.2915	0.1802
Fe	Fe22	0.0584	0.2915	0.1802
Fe	Fe23	0.5584	0.7915	0.1802
Fe	Fe24	0.0584	0.7915	0.1802
Fe	Fe25	0.2085	0.9915	0.2162
Fe	Fe26	0.7085	0.9915	0.2162
Fe	Fe27	0.7085	0.4915	0.2162
Fe	Fe28	0.2085	0.4915	0.2162
Fe	Fe29	0.3584	0.1915	0.2523

Fe	Fe30	0.8584	0.6915	0.2523
Fe	Fe31	0.8584	0.1915	0.2523
Fe	Fe32	0.3584	0.6915	0.2523
Fe	Fe33	0.0090467207514364	0.8900186837884136	0.2890554954170461
Fe	Fe34	0.0088599868058597	0.3903944357089005	0.2890033266986852
Fe	Fe35	0.5089402117691905	0.3903991791926842	0.2890089680703990
Fe	Fe36	0.5090792621750166	0.8899434659956627	0.2886433247173423
Fe	Fe37	0.6579544792765789	0.0911411105066313	0.3240548974982952
Fe	Fe38	0.1587973322932749	0.0911369913748243	0.3240511776380766
Fe	Fe39	0.6577329371661229	0.5926069396987989	0.3248793225557621
Fe	Fe40	0.1575033973658299	0.5929258682778816	0.3245785868555792
Fe	Fe41	0.3046431560320504	0.7920936942966358	0.3633926959614425
Fe	Fe42	0.8112354277645303	0.7920548317699734	0.3634201516695373
Fe	Fe43	0.8115712986910862	0.2850131281528310	0.3649142028348202
Fe	Fe44	0.3070765670248155	0.2937266657483724	0.3614033176954903
Fe	Fe45	0.9608450665889493	0.5010292284120528	0.3963982933592530
Fe	Fe46	0.4459377581854830	0.5011132869575923	0.3963543755223809
Fe	Fe47	0.4551909752549652	-0.0025251614796412	0.3936695197565824
Fe	Fe48	0.9498053529736256	0.0081230032257645	0.3954877069205840
N	N49	0.7527707953516539	0.4019632921614306	0.4346085265562638
H	H50	0.8315572314357526	0.2440244245047832	0.4287089238189423
H	H51	0.7585940391901564	0.3897354589481185	0.4757259521889025

7.10 H_2N+H hydrogenation.cif

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_cell_angle_gamma 72.4516

_symmetry_space_group_name_H-M 'T'

loop_

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_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe	Fe1	0.8084	0.2915	0.0000
Fe	Fe2	0.3085	0.2915	0.0000
Fe	Fe3	0.3085	0.7915	0.0000
Fe	Fe4	0.8084	0.7915	0.0000
Fe	Fe5	0.9585	0.9915	0.0360
Fe	Fe6	0.4584	0.9915	0.0360
Fe	Fe7	0.9585	0.4915	0.0360
Fe	Fe8	0.4584	0.4915	0.0360
Fe	Fe9	0.1085	0.6915	0.0721
Fe	Fe10	0.6084	0.6915	0.0721
Fe	Fe11	0.1085	0.1915	0.0721
Fe	Fe12	0.6084	0.1915	0.0721
Fe	Fe13	0.2585	0.8915	0.1081
Fe	Fe14	0.7584	0.8915	0.1081
Fe	Fe15	0.2585	0.3915	0.1081
Fe	Fe16	0.7584	0.3915	0.1081
Fe	Fe17	0.9085	0.0915	0.1442
Fe	Fe18	0.4085	0.0915	0.1442
Fe	Fe19	0.4085	0.5915	0.1442
Fe	Fe20	0.9085	0.5915	0.1442
Fe	Fe21	0.5584	0.2915	0.1802
Fe	Fe22	0.0584	0.2915	0.1802
Fe	Fe23	0.5584	0.7915	0.1802

Fe	Fe24	0.0584	0.7915	0.1802
Fe	Fe25	0.2085	0.9915	0.2162
Fe	Fe26	0.7085	0.9915	0.2162
Fe	Fe27	0.7085	0.4915	0.2162
Fe	Fe28	0.2085	0.4915	0.2162
Fe	Fe29	0.3584	0.1915	0.2523
Fe	Fe30	0.8584	0.6915	0.2523
Fe	Fe31	0.8584	0.1915	0.2523
Fe	Fe32	0.3584	0.6915	0.2523
Fe	Fe33	0.0105950574648461	0.8902390153884765	0.2892083691858047
Fe	Fe34	0.0094828759843348	0.3892057026403394	0.2888186360906632
Fe	Fe35	0.5091059764523049	0.3899543086640027	0.2892919990869332
Fe	Fe36	0.5074653621902075	0.8902096756888345	0.2892106394257994
Fe	Fe37	0.6577765423942608	0.0924945602777212	0.3247408875834600
Fe	Fe38	0.1574815970714446	0.0931627966068620	0.3250405635672408
Fe	Fe39	0.6573946261781637	0.5923376085175530	0.3239173665126892
Fe	Fe40	0.1582865679632301	0.5923330537930681	0.3239148406548732
Fe	Fe41	0.3076793518199333	0.7927655039718911	0.3657137639686563
Fe	Fe42	0.8072144851165537	0.7936924575993287	0.3619388273157862
Fe	Fe43	0.8024830245876772	0.2928643488599670	0.3637411133877563
Fe	Fe44	0.3126894954551198	0.2927647731904582	0.3637733420818163
Fe	Fe45	0.9557393681168306	0.4966260153060096	0.3924056656504964
Fe	Fe46	0.4486937763204411	0.5104559244590399	0.3968473244155804
Fe	Fe47	0.4557495205334814	0.0024454687447061	0.3954146243621848
Fe	Fe48	0.9497259323975394	0.0025457203101401	0.3953805771569210
N	N49	0.3617181622816931	0.6858509802497346	0.4492135956584155
H	H50	0.2852323280163629	0.8390750255854112	0.4326293135793646
H	H51	0.2128742191300382	0.6899985279872345	0.4734621722899688
H	H52	0.5072062890842255	0.6898364606482383	0.4732486626718844

8. (311) surface

8.1 H adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 13.8740
_cell_length_b 8.0101
_cell_length_c 21.4041
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 106.7786

_symmetry_space_group_name_H-M 'T'

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
Fe Fe1 0.2800 0.1687 0.0000
Fe Fe2 0.7800 0.6687 0.0000
Fe Fe3 0.2800 0.6687 0.0000
Fe Fe4 0.7800 0.1687 0.0000
Fe Fe5 0.4618 0.7596 0.0200
Fe Fe6 0.9618 0.2596 0.0200
Fe Fe7 0.9618 0.7596 0.0200
Fe Fe8 0.4618 0.2596 0.0200
Fe Fe9 0.6436 0.3505 0.0399
Fe Fe10 0.1436 0.8505 0.0399
Fe Fe11 0.6436 0.8505 0.0399
Fe Fe12 0.1436 0.3505 0.0399
Fe Fe13 0.3255 0.4414 0.0598
Fe Fe14 0.8255 0.9414 0.0598

Fe	Fe15	0.8255	0.4414	0.0598
Fe	Fe16	0.3255	0.9414	0.0598
Fe	Fe17	0.0073	0.0323	0.0798
Fe	Fe18	0.5073	0.0323	0.0798
Fe	Fe19	0.0073	0.5323	0.0798
Fe	Fe20	0.5073	0.5323	0.0798
Fe	Fe21	0.6891	0.1232	0.0997
Fe	Fe22	0.1891	0.6232	0.0997
Fe	Fe23	0.1891	0.1232	0.0997
Fe	Fe24	0.6891	0.6232	0.0997
Fe	Fe25	0.3709	0.2141	0.1197
Fe	Fe26	0.8709	0.2141	0.1197
Fe	Fe27	0.8709	0.7141	0.1197
Fe	Fe28	0.3709	0.7141	0.1197
Fe	Fe29	0.0527	0.8050	0.1396
Fe	Fe30	0.5527	0.8050	0.1396
Fe	Fe31	0.5527	0.3050	0.1396
Fe	Fe32	0.0527	0.3050	0.1396
Fe	Fe33	0.2345	0.8959	0.1596
Fe	Fe34	0.2345	0.3959	0.1596
Fe	Fe35	0.7345	0.8959	0.1596
Fe	Fe36	0.7345	0.3959	0.1596
Fe	Fe37	0.9164	0.4868	0.1795
Fe	Fe38	0.4164	0.4868	0.1795
Fe	Fe39	0.4164	0.9868	0.1795
Fe	Fe40	0.9164	0.9868	0.1795
Fe	Fe41	0.0993799335122369	0.5783595865775083	0.1995348906010407
Fe	Fe42	0.5995163005515745	0.5776853623520426	0.1989394171284586
Fe	Fe43	0.5995381664940980	0.0791665679895317	0.1989342817716881
Fe	Fe44	0.0992791207557053	0.0783022355698793	0.1994136008345786
Fe	Fe45	0.2804293089459762	0.6689252819760798	0.2236700271308760
Fe	Fe46	0.7790380357585300	0.1678777203235880	0.2237347383043339
Fe	Fe47	0.7790298784716496	0.6685942861314619	0.2237251386158292

Fe	Fe48	0.2799534541063946	0.1686992981938357	0.2232547122108847
Fe	Fe49	0.4637309734056842	0.2605676411710419	0.2427258271420825
Fe	Fe50	0.9627253273911350	0.7602232048094509	0.2428999164081390
Fe	Fe51	0.9627425356595132	0.2599080792605470	0.2429029118125285
Fe	Fe52	0.4634638228530744	0.7604091548460814	0.2430564842628975
Fe	Fe53	0.1496658711366831	0.8537049953206056	0.2607916210730846
Fe	Fe54	0.1496685752961109	0.3532694361016256	0.2607951146379789
Fe	Fe55	0.6505919326091912	0.8539027257763677	0.2620588533210605
Fe	Fe56	0.6487203122611418	0.3529695338628494	0.2616493209310208
Fe	Fe57	0.8384574238713604	0.4479729085324389	0.2797435559109872
Fe	Fe58	0.3372474486886505	0.4451546779560990	0.2798648504764675
Fe	Fe59	0.8382391503984343	0.9478375053778324	0.2799171034544205
Fe	Fe60	0.3372506399895193	0.9495343330855722	0.2798618507910028
Fe	Fe61	0.5287931387018552	0.0445495983032218	0.2964839581994843
Fe	Fe62	0.0287802923485512	0.0431406974485363	0.2974595164274783
Fe	Fe63	0.0281244600932744	0.5428184201990612	0.2974069255633358
Fe	Fe64	0.5288330380599650	0.5417439980305461	0.2964817807284804
H	H65	0.5401618760404400	0.7985815291193366	0.3109717277275217

8.2 N adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 13.8740
_cell_length_b 8.0101
_cell_length_c 21.4041
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 106.7786

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.7800	0.6687	0.0000
Fe	Fe3	0.2800	0.6687	0.0000
Fe	Fe4	0.7800	0.1687	0.0000
Fe	Fe5	0.4618	0.7596	0.0200
Fe	Fe6	0.9618	0.2596	0.0200
Fe	Fe7	0.9618	0.7596	0.0200
Fe	Fe8	0.4618	0.2596	0.0200
Fe	Fe9	0.6436	0.3505	0.0399
Fe	Fe10	0.1436	0.8505	0.0399
Fe	Fe11	0.6436	0.8505	0.0399
Fe	Fe12	0.1436	0.3505	0.0399
Fe	Fe13	0.3255	0.4414	0.0598
Fe	Fe14	0.8255	0.9414	0.0598
Fe	Fe15	0.8255	0.4414	0.0598
Fe	Fe16	0.3255	0.9414	0.0598
Fe	Fe17	0.0073	0.0323	0.0798
Fe	Fe18	0.5073	0.0323	0.0798
Fe	Fe19	0.0073	0.5323	0.0798
Fe	Fe20	0.5073	0.5323	0.0798
Fe	Fe21	0.6891	0.1232	0.0997
Fe	Fe22	0.1891	0.6232	0.0997
Fe	Fe23	0.1891	0.1232	0.0997
Fe	Fe24	0.6891	0.6232	0.0997
Fe	Fe25	0.3709	0.2141	0.1197
Fe	Fe26	0.8709	0.2141	0.1197
Fe	Fe27	0.8709	0.7141	0.1197

Fe	Fe28	0.3709	0.7141	0.1197
Fe	Fe29	0.0527	0.8050	0.1396
Fe	Fe30	0.5527	0.8050	0.1396
Fe	Fe31	0.5527	0.3050	0.1396
Fe	Fe32	0.0527	0.3050	0.1396
Fe	Fe33	0.2345	0.8959	0.1596
Fe	Fe34	0.2345	0.3959	0.1596
Fe	Fe35	0.7345	0.8959	0.1596
Fe	Fe36	0.7345	0.3959	0.1596
Fe	Fe37	0.9164	0.4868	0.1795
Fe	Fe38	0.4164	0.4868	0.1795
Fe	Fe39	0.4164	0.9868	0.1795
Fe	Fe40	0.9164	0.9868	0.1795
Fe	Fe41	0.0984	0.5778	0.1993
Fe	Fe42	0.5992	0.5763	0.2004
Fe	Fe43	0.5992	0.0801	0.2004
Fe	Fe44	0.0989	0.0781	0.1994
Fe	Fe45	0.2769	0.6671	0.2242
Fe	Fe46	0.7791	0.1688	0.2227
Fe	Fe47	0.7791	0.6678	0.2227
Fe	Fe48	0.2794	0.1684	0.2228
Fe	Fe49	0.4636	0.2605	0.2435
Fe	Fe50	0.9622	0.7596	0.2429
Fe	Fe51	0.9622	0.2600	0.2429
Fe	Fe52	0.4576	0.7574	0.2398
Fe	Fe53	0.1473	0.8539	0.2609
Fe	Fe54	0.1473	0.3507	0.2609
Fe	Fe55	0.6537	0.8554	0.2593
Fe	Fe56	0.6466	0.3519	0.2619
Fe	Fe57	0.8371	0.4473	0.2794
Fe	Fe58	0.3370	0.4416	0.2794
Fe	Fe59	0.8362	0.9468	0.2795
Fe	Fe60	0.3370	0.9528	0.2794

Fe Fe61 0.5213 0.0235 0.2987

Fe Fe62 0.0274 0.0424 0.2974

Fe Fe63 0.0287 0.5431 0.2974

Fe Fe64 0.5212 0.5549 0.2987

N N65 0.5426 0.7999 0.3100

8.3 N_2 adsorption.cif

data_

_audit_creation_method 'generated by wxDragon 1.3.4 '

_cell_length_a 13.8740

_cell_length_b 8.0101

_cell_length_c 21.4041

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 106.7786

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

Fe Fe1 0.2800 0.1687 0.0000

Fe Fe2 0.7800 0.6687 0.0000

Fe Fe3 0.2800 0.6687 0.0000

Fe Fe4 0.7800 0.1687 0.0000

Fe Fe5 0.4618 0.7596 0.0200

Fe Fe6 0.9618 0.2596 0.0200

Fe Fe7 0.9618 0.7596 0.0200

Fe	Fe8	0.4618	0.2596	0.0200
Fe	Fe9	0.6436	0.3505	0.0399
Fe	Fe10	0.1436	0.8505	0.0399
Fe	Fe11	0.6436	0.8505	0.0399
Fe	Fe12	0.1436	0.3505	0.0399
Fe	Fe13	0.3255	0.4414	0.0598
Fe	Fe14	0.8255	0.9414	0.0598
Fe	Fe15	0.8255	0.4414	0.0598
Fe	Fe16	0.3255	0.9414	0.0598
Fe	Fe17	0.0073	0.0323	0.0798
Fe	Fe18	0.5073	0.0323	0.0798
Fe	Fe19	0.0073	0.5323	0.0798
Fe	Fe20	0.5073	0.5323	0.0798
Fe	Fe21	0.6891	0.1232	0.0997
Fe	Fe22	0.1891	0.6232	0.0997
Fe	Fe23	0.1891	0.1232	0.0997
Fe	Fe24	0.6891	0.6232	0.0997
Fe	Fe25	0.3709	0.2141	0.1197
Fe	Fe26	0.8709	0.2141	0.1197
Fe	Fe27	0.8709	0.7141	0.1197
Fe	Fe28	0.3709	0.7141	0.1197
Fe	Fe29	0.0527	0.8050	0.1396
Fe	Fe30	0.5527	0.8050	0.1396
Fe	Fe31	0.5527	0.3050	0.1396
Fe	Fe32	0.0527	0.3050	0.1396
Fe	Fe33	0.2345	0.8959	0.1596
Fe	Fe34	0.2345	0.3959	0.1596
Fe	Fe35	0.7345	0.8959	0.1596
Fe	Fe36	0.7345	0.3959	0.1596
Fe	Fe37	0.9164	0.4868	0.1795
Fe	Fe38	0.4164	0.4868	0.1795
Fe	Fe39	0.4164	0.9868	0.1795
Fe	Fe40	0.9164	0.9868	0.1795

Fe	Fe41	0.0965997116531359	0.5770342261917889	0.1979307525262171
Fe	Fe42	0.5991439855229005	0.5780931396787475	0.1998472577613698
Fe	Fe43	0.5991516860600187	0.0784037014266328	0.1998501578225985
Fe	Fe44	0.0998879304219783	0.0786533876356649	0.2000926688903876
Fe	Fe45	0.2821521232032707	0.6698120969974828	0.2195695507123820
Fe	Fe46	0.7794915450533512	0.1684036808494582	0.2234234047636187
Fe	Fe47	0.7794854585465406	0.6685701899133328	0.2234260142273058
Fe	Fe48	0.2790075179605499	0.1682269657701503	0.2255106700518534
Fe	Fe49	0.4618841242903491	0.2596493758668298	0.2431800768237846
Fe	Fe50	0.9629707810013063	0.7614948224759397	0.2422716650808714
Fe	Fe51	0.9629549368558057	0.2589428721139959	0.2422531187578446
Fe	Fe52	0.4661474251451129	0.7617542113357698	0.2412731674110856
Fe	Fe53	0.1490023666709845	0.8439035119282794	0.2627621974911767
Fe	Fe54	0.1489856880520573	0.3626605396283147	0.2627640327024395
Fe	Fe55	0.6507937480092523	0.8540529119206104	0.2610220973368929
Fe	Fe56	0.6486135547543417	0.3529509110362696	0.2608679654707389
Fe	Fe57	0.8365271565734208	0.4470378302682696	0.2797682685408346
Fe	Fe58	0.3395674103475051	0.4532657227541235	0.2821181055783303
Fe	Fe59	0.8387494594449345	0.9481364371149422	0.2800616304129131
Fe	Fe60	0.3396206547651096	0.9437699239764367	0.2821292172015865
Fe	Fe61	0.5239162133215320	0.0400478588707371	0.2973871403520827
Fe	Fe62	0.0301302223880520	0.0439327441673323	0.2970755804794962
Fe	Fe63	0.0227149458181644	0.5401521492021457	0.2971418219821519
Fe	Fe64	0.5239155184302045	0.5413690024304484	0.2973817715948146
N	N65	0.2360967908838410	0.7287967966477712	0.3061863515835790
N	N66	0.2360663471131538	0.5647447967026311	0.3061997909929749

8.4 NH adsorption.cif

data_

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_cell_length_b 8.0101

_cell_length_c 21.4041

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 106.7786

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.7800	0.6687	0.0000
Fe	Fe3	0.2800	0.6687	0.0000
Fe	Fe4	0.7800	0.1687	0.0000
Fe	Fe5	0.4618	0.7596	0.0200
Fe	Fe6	0.9618	0.2596	0.0200
Fe	Fe7	0.9618	0.7596	0.0200
Fe	Fe8	0.4618	0.2596	0.0200
Fe	Fe9	0.6436	0.3505	0.0399
Fe	Fe10	0.1436	0.8505	0.0399
Fe	Fe11	0.6436	0.8505	0.0399
Fe	Fe12	0.1436	0.3505	0.0399
Fe	Fe13	0.3255	0.4414	0.0598
Fe	Fe14	0.8255	0.9414	0.0598
Fe	Fe15	0.8255	0.4414	0.0598
Fe	Fe16	0.3255	0.9414	0.0598
Fe	Fe17	0.0073	0.0323	0.0798
Fe	Fe18	0.5073	0.0323	0.0798
Fe	Fe19	0.0073	0.5323	0.0798

Fe	Fe20	0.5073	0.5323	0.0798
Fe	Fe21	0.6891	0.1232	0.0997
Fe	Fe22	0.1891	0.6232	0.0997
Fe	Fe23	0.1891	0.1232	0.0997
Fe	Fe24	0.6891	0.6232	0.0997
Fe	Fe25	0.3709	0.2141	0.1197
Fe	Fe26	0.8709	0.2141	0.1197
Fe	Fe27	0.8709	0.7141	0.1197
Fe	Fe28	0.3709	0.7141	0.1197
Fe	Fe29	0.0527	0.8050	0.1396
Fe	Fe30	0.5527	0.8050	0.1396
Fe	Fe31	0.5527	0.3050	0.1396
Fe	Fe32	0.0527	0.3050	0.1396
Fe	Fe33	0.2345	0.8959	0.1596
Fe	Fe34	0.2345	0.3959	0.1596
Fe	Fe35	0.7345	0.8959	0.1596
Fe	Fe36	0.7345	0.3959	0.1596
Fe	Fe37	0.9164	0.4868	0.1795
Fe	Fe38	0.4164	0.4868	0.1795
Fe	Fe39	0.4164	0.9868	0.1795
Fe	Fe40	0.9164	0.9868	0.1795
Fe	Fe41	0.0985088384553824	0.5779038214424809	0.1994255813245381
Fe	Fe42	0.5994824805126859	0.5782801705950241	0.2001384634012384
Fe	Fe43	0.5994713880659316	0.0785290729481125	0.2001455047412657
Fe	Fe44	0.0988424800708095	0.0780833093373154	0.1991251299701343
Fe	Fe45	0.2772775253771271	0.6672798134360904	0.2245608034961455
Fe	Fe46	0.7796065046735116	0.1689814481131157	0.2229943037008001
Fe	Fe47	0.7796091552868658	0.6680725916470824	0.2229907881277760
Fe	Fe48	0.2788778944708203	0.1681580829227433	0.2226919055468553
Fe	Fe49	0.4636038292122227	0.2604402964277782	0.2423093017344994
Fe	Fe50	0.9624952737671636	0.7596931058246450	0.2430182826523098
Fe	Fe51	0.9624936390970994	0.2601960112288943	0.2430125024049666
Fe	Fe52	0.4576757287447495	0.7574599495956523	0.2422750188024262

Fe	Fe53	0.1474434185525131	0.8535441855476790	0.2608171276583579
Fe	Fe54	0.1474510605330587	0.3511616382191230	0.2608245429437881
Fe	Fe55	0.6557825704948409	0.8565494767821634	0.2615691958086346
Fe	Fe56	0.6473718449635010	0.3522976165802097	0.2617365465776841
Fe	Fe57	0.8374129108195557	0.4474663975999764	0.2796715479741929
Fe	Fe58	0.3357238992972134	0.4393512269891540	0.2798763901816593
Fe	Fe59	0.8385319425686685	0.9480039646251093	0.2796491094826911
Fe	Fe60	0.3357072873153837	0.9536677537398361	0.2798480707257800
Fe	Fe61	0.5204429220276285	0.0337746607403146	0.2972575075658211
Fe	Fe62	0.0288930457428405	0.0432249944397868	0.2973285360415878
Fe	Fe63	0.0289254228441555	0.5432083688296763	0.2976249475102069
Fe	Fe64	0.5204820396396386	0.5439820970589759	0.2972420980838218
N	N65	0.5449134848278891	0.8010632207669235	0.3194624740437417
H	H66	0.5390336921709934	0.7980979633064214	0.3675423221293670

8.5 NH_2 adsorption.cif

data_

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_cell_length_c 21.4041
_cell_angle_alpha 90.0000
_cell_angle_beta 90.0000
_cell_angle_gamma 106.7786

_symmetry_space_group_name_H-M 'T'

loop_
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_atom_site_label
_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe2	0.7800	0.6687	0.0000
Fe	Fe3	0.2800	0.6687	0.0000
Fe	Fe4	0.7800	0.1687	0.0000
Fe	Fe5	0.4618	0.7596	0.0200
Fe	Fe6	0.9618	0.2596	0.0200
Fe	Fe7	0.9618	0.7596	0.0200
Fe	Fe8	0.4618	0.2596	0.0200
Fe	Fe9	0.6436	0.3505	0.0399
Fe	Fe10	0.1436	0.8505	0.0399
Fe	Fe11	0.6436	0.8505	0.0399
Fe	Fe12	0.1436	0.3505	0.0399
Fe	Fe13	0.3255	0.4414	0.0598
Fe	Fe14	0.8255	0.9414	0.0598
Fe	Fe15	0.8255	0.4414	0.0598
Fe	Fe16	0.3255	0.9414	0.0598
Fe	Fe17	0.0073	0.0323	0.0798
Fe	Fe18	0.5073	0.0323	0.0798
Fe	Fe19	0.0073	0.5323	0.0798
Fe	Fe20	0.5073	0.5323	0.0798
Fe	Fe21	0.6891	0.1232	0.0997
Fe	Fe22	0.1891	0.6232	0.0997
Fe	Fe23	0.1891	0.1232	0.0997
Fe	Fe24	0.6891	0.6232	0.0997
Fe	Fe25	0.3709	0.2141	0.1197
Fe	Fe26	0.8709	0.2141	0.1197
Fe	Fe27	0.8709	0.7141	0.1197
Fe	Fe28	0.3709	0.7141	0.1197
Fe	Fe29	0.0527	0.8050	0.1396
Fe	Fe30	0.5527	0.8050	0.1396
Fe	Fe31	0.5527	0.3050	0.1396

Fe	Fe32	0.0527	0.3050	0.1396
Fe	Fe33	0.2345	0.8959	0.1596
Fe	Fe34	0.2345	0.3959	0.1596
Fe	Fe35	0.7345	0.8959	0.1596
Fe	Fe36	0.7345	0.3959	0.1596
Fe	Fe37	0.9164	0.4868	0.1795
Fe	Fe38	0.4164	0.4868	0.1795
Fe	Fe39	0.4164	0.9868	0.1795
Fe	Fe40	0.9164	0.9868	0.1795
Fe	Fe41	0.0989633231016353	0.5780082968793390	0.1995413797721125
Fe	Fe42	0.5983791741238985	0.5778294811642107	0.2000544229156183
Fe	Fe43	0.5994092297794894	0.0784369396665667	0.1991922520143570
Fe	Fe44	0.0989753610630663	0.0782950012062007	0.1995628127531079
Fe	Fe45	0.2788658732498647	0.6667841327564685	0.2239243084917200
Fe	Fe46	0.7790831130110798	0.1682558162929066	0.2236517290720533
Fe	Fe47	0.7775884349464223	0.6675092519382825	0.2237591653970662
Fe	Fe48	0.2788634541793455	0.1696857323167862	0.2239454506564057
Fe	Fe49	0.4631229462109493	0.2604980407634818	0.2417492642666897
Fe	Fe50	0.9620219982562186	0.7596725175942700	0.2425491409718906
Fe	Fe51	0.9621996063413303	0.2597689900044136	0.2426948497200598
Fe	Fe52	0.4631381665323223	0.7602138654226045	0.2416291391757591
Fe	Fe53	0.1492012797188146	0.8532377952772984	0.2606840354458480
Fe	Fe54	0.1492523796354885	0.3532710665437354	0.2612471643692011
Fe	Fe55	0.6486140571509527	0.8522719370232702	0.2610531244919952
Fe	Fe56	0.6485683412124247	0.3536533130114541	0.2610827259003528
Fe	Fe57	0.8370705919740186	0.4472329237410709	0.2798530952050906
Fe	Fe58	0.3377880266989436	0.4479180318546568	0.2832421732807588
Fe	Fe59	0.8370607934941160	0.9472794585539834	0.2798663440112011
Fe	Fe60	0.3373697427372701	0.9475100978737228	0.2794996300000807
Fe	Fe61	0.5274009919667693	0.0424646763731553	0.2964487705810772
Fe	Fe62	0.0270102726413384	0.0422868581159097	0.2971153493825146
Fe	Fe63	0.0270529514852012	0.5421265768437518	0.2971260331569002
Fe	Fe64	0.5265995634946472	0.5425634447303816	0.3007073568651317

N	N65	0.4141600751849158	0.4890125157751611	0.3625461880902541
H	H66	0.4080244179263650	0.3831742509607192	0.3907847498321361
H	H67	0.4081143313244951	0.5914622049361212	0.3893619725206651

8.6 NH_3 adsorption.cif

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_cell_length_c 21.4041
_cell_angle_alpha 90.0000
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_cell_angle_gamma 106.7786

_symmetry_space_group_name_H-M 'T'

loop_
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_atom_site_label
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Fe	Fe2	0.7800	0.6687	0.0000
Fe	Fe3	0.2800	0.6687	0.0000
Fe	Fe4	0.7800	0.1687	0.0000
Fe	Fe5	0.4618	0.7596	0.0200
Fe	Fe6	0.9618	0.2596	0.0200
Fe	Fe7	0.9618	0.7596	0.0200
Fe	Fe8	0.4618	0.2596	0.0200
Fe	Fe9	0.6436	0.3505	0.0399

Fe	Fe10	0.1436	0.8505	0.0399
Fe	Fe11	0.6436	0.8505	0.0399
Fe	Fe12	0.1436	0.3505	0.0399
Fe	Fe13	0.3255	0.4414	0.0598
Fe	Fe14	0.8255	0.9414	0.0598
Fe	Fe15	0.8255	0.4414	0.0598
Fe	Fe16	0.3255	0.9414	0.0598
Fe	Fe17	0.0073	0.0323	0.0798
Fe	Fe18	0.5073	0.0323	0.0798
Fe	Fe19	0.0073	0.5323	0.0798
Fe	Fe20	0.5073	0.5323	0.0798
Fe	Fe21	0.6891	0.1232	0.0997
Fe	Fe22	0.1891	0.6232	0.0997
Fe	Fe23	0.1891	0.1232	0.0997
Fe	Fe24	0.6891	0.6232	0.0997
Fe	Fe25	0.3709	0.2141	0.1197
Fe	Fe26	0.8709	0.2141	0.1197
Fe	Fe27	0.8709	0.7141	0.1197
Fe	Fe28	0.3709	0.7141	0.1197
Fe	Fe29	0.0527	0.8050	0.1396
Fe	Fe30	0.5527	0.8050	0.1396
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Fe	Fe34	0.2345	0.3959	0.1596
Fe	Fe35	0.7345	0.8959	0.1596
Fe	Fe36	0.7345	0.3959	0.1596
Fe	Fe37	0.9164	0.4868	0.1795
Fe	Fe38	0.4164	0.4868	0.1795
Fe	Fe39	0.4164	0.9868	0.1795
Fe	Fe40	0.9164	0.9868	0.1795
Fe	Fe41	0.0991497048937889	0.5784120687580883	0.1995846059563643
Fe	Fe42	0.5985816930165396	0.5779455228334225	0.1996499262618898

Fe	Fe43	0.5991623060867864	0.0782226509979672	0.1993404698433769
Fe	Fe44	0.0991509644599318	0.0780759854205780	0.1995886858741530
Fe	Fe45	0.2791220163787511	0.6685041257263389	0.2236263180500098
Fe	Fe46	0.7791904249570353	0.1683141104257662	0.2236769577550449
Fe	Fe47	0.7786127224568563	0.6680435190875093	0.2237958633720112
Fe	Fe48	0.2791027399669795	0.1680796762056233	0.2236539040403976
Fe	Fe49	0.4628150259068944	0.2611158918500712	0.2430460207628475
Fe	Fe50	0.9625430983473454	0.7599812230007105	0.2428945247783160
Fe	Fe51	0.9627626186802387	0.2600547485373352	0.2428697520170803
Fe	Fe52	0.4628258164374288	0.7590359283764954	0.2430853326003364
Fe	Fe53	0.1495548042848536	0.8533870600676643	0.2612725275281897
Fe	Fe54	0.1491859315045682	0.3532696703493119	0.2612071760258968
Fe	Fe55	0.6491837977510796	0.8527524541721401	0.2607770010884746
Fe	Fe56	0.6492145385975810	0.3536855320075717	0.2607491628138738
Fe	Fe57	0.8377182990788786	0.4473513610002608	0.2797071307106406
Fe	Fe58	0.3375798104048424	0.4475684009057370	0.2790040808256362
Fe	Fe59	0.8376818938050867	0.9478818835320461	0.2797153713327487
Fe	Fe60	0.3382176944553022	0.9478198159823261	0.2798821611827053
Fe	Fe61	0.5277762177633873	0.0426762597243108	0.2966911353680622
Fe	Fe62	0.0278298231185688	0.0424303923978913	0.2973595759987902
Fe	Fe63	0.0277928858882294	0.5427742027209739	0.2973605958692594
Fe	Fe64	0.5298768061289371	0.5434937920063968	0.3003983119347531
N	N65	0.5375951215502554	0.5479199641444616	0.3989257829976092
H	H66	0.5031281749137411	0.4267606101872511	0.4169014957869216
H	H67	0.5028040742731694	0.6344102169132019	0.4166858501627831
H	H68	0.6109993107169882	0.5850601787913329	0.4136567030171300

8.7 N_2 activation.cif

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_cell_length_b 8.0101

_cell_length_c 21.4041

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 106.7786

_symmetry_space_group_name_H-M 'T'

loop_

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Fe	Fe2	0.7800	0.6687	0.0000
Fe	Fe3	0.2800	0.6687	0.0000
Fe	Fe4	0.7800	0.1687	0.0000
Fe	Fe5	0.4618	0.7596	0.0200
Fe	Fe6	0.9618	0.2596	0.0200
Fe	Fe7	0.9618	0.7596	0.0200
Fe	Fe8	0.4618	0.2596	0.0200
Fe	Fe9	0.6436	0.3505	0.0399
Fe	Fe10	0.1436	0.8505	0.0399
Fe	Fe11	0.6436	0.8505	0.0399
Fe	Fe12	0.1436	0.3505	0.0399
Fe	Fe13	0.3255	0.4414	0.0598
Fe	Fe14	0.8255	0.9414	0.0598
Fe	Fe15	0.8255	0.4414	0.0598
Fe	Fe16	0.3255	0.9414	0.0598
Fe	Fe17	0.0073	0.0323	0.0798
Fe	Fe18	0.5073	0.0323	0.0798
Fe	Fe19	0.0073	0.5323	0.0798

Fe	Fe20	0.5073	0.5323	0.0798
Fe	Fe21	0.6891	0.1232	0.0997
Fe	Fe22	0.1891	0.6232	0.0997
Fe	Fe23	0.1891	0.1232	0.0997
Fe	Fe24	0.6891	0.6232	0.0997
Fe	Fe25	0.3709	0.2141	0.1197
Fe	Fe26	0.8709	0.2141	0.1197
Fe	Fe27	0.8709	0.7141	0.1197
Fe	Fe28	0.3709	0.7141	0.1197
Fe	Fe29	0.0527	0.8050	0.1396
Fe	Fe30	0.5527	0.8050	0.1396
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Fe	Fe32	0.0527	0.3050	0.1396
Fe	Fe33	0.2345	0.8959	0.1596
Fe	Fe34	0.2345	0.3959	0.1596
Fe	Fe35	0.7345	0.8959	0.1596
Fe	Fe36	0.7345	0.3959	0.1596
Fe	Fe37	0.9164	0.4868	0.1795
Fe	Fe38	0.4164	0.4868	0.1795
Fe	Fe39	0.4164	0.9868	0.1795
Fe	Fe40	0.9164	0.9868	0.1795
Fe	Fe41	0.0962	0.5768	0.1977
Fe	Fe42	0.5988	0.5781	0.1999
Fe	Fe43	0.5988	0.0780	0.1999
Fe	Fe44	0.0995	0.0785	0.1997
Fe	Fe45	0.2790	0.6682	0.2242
Fe	Fe46	0.7789	0.1682	0.2232
Fe	Fe47	0.7789	0.6682	0.2232
Fe	Fe48	0.2790	0.1683	0.2248
Fe	Fe49	0.4632	0.2603	0.2423
Fe	Fe50	0.9615	0.7602	0.2426
Fe	Fe51	0.9615	0.2587	0.2426
Fe	Fe52	0.4642	0.7607	0.2419

Fe	Fe53	0.1470	0.8468	0.2614
Fe	Fe54	0.1469	0.3575	0.2614
Fe	Fe55	0.6493	0.8532	0.2607
Fe	Fe56	0.6486	0.3529	0.2608
Fe	Fe57	0.8363	0.4469	0.2799
Fe	Fe58	0.3410	0.4463	0.2815
Fe	Fe59	0.8368	0.9472	0.2797
Fe	Fe60	0.3410	0.9521	0.2815
Fe	Fe61	0.5229	0.0419	0.2978
Fe	Fe62	0.0289	0.0433	0.2969
Fe	Fe63	0.0251	0.5414	0.2971
Fe	Fe64	0.5228	0.5383	0.2978
N	N65	0.2369	0.5355	0.3021
N	N66	0.2369	0.7587	0.3021

8.8 N+H hydrogenation.cif

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_cell_length_c 21.4041

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 106.7786

_symmetry_space_group_name_H-M 'T'

loop_

_atom_site_type_symbol

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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Fe	Fe3	0.2800	0.6687	0.0000
Fe	Fe4	0.7800	0.1687	0.0000
Fe	Fe5	0.4618	0.7596	0.0200
Fe	Fe6	0.9618	0.2596	0.0200
Fe	Fe7	0.9618	0.7596	0.0200
Fe	Fe8	0.4618	0.2596	0.0200
Fe	Fe9	0.6436	0.3505	0.0399
Fe	Fe10	0.1436	0.8505	0.0399
Fe	Fe11	0.6436	0.8505	0.0399
Fe	Fe12	0.1436	0.3505	0.0399
Fe	Fe13	0.3255	0.4414	0.0598
Fe	Fe14	0.8255	0.9414	0.0598
Fe	Fe15	0.8255	0.4414	0.0598
Fe	Fe16	0.3255	0.9414	0.0598
Fe	Fe17	0.0073	0.0323	0.0798
Fe	Fe18	0.5073	0.0323	0.0798
Fe	Fe19	0.0073	0.5323	0.0798
Fe	Fe20	0.5073	0.5323	0.0798
Fe	Fe21	0.6891	0.1232	0.0997
Fe	Fe22	0.1891	0.6232	0.0997
Fe	Fe23	0.1891	0.1232	0.0997
Fe	Fe24	0.6891	0.6232	0.0997
Fe	Fe25	0.3709	0.2141	0.1197
Fe	Fe26	0.8709	0.2141	0.1197
Fe	Fe27	0.8709	0.7141	0.1197
Fe	Fe28	0.3709	0.7141	0.1197
Fe	Fe29	0.0527	0.8050	0.1396
Fe	Fe30	0.5527	0.8050	0.1396
Fe	Fe31	0.5527	0.3050	0.1396

Fe	Fe32	0.0527	0.3050	0.1396
Fe	Fe33	0.2345	0.8959	0.1596
Fe	Fe34	0.2345	0.3959	0.1596
Fe	Fe35	0.7345	0.8959	0.1596
Fe	Fe36	0.7345	0.3959	0.1596
Fe	Fe37	0.9164	0.4868	0.1795
Fe	Fe38	0.4164	0.4868	0.1795
Fe	Fe39	0.4164	0.9868	0.1795
Fe	Fe40	0.9164	0.9868	0.1795
Fe	Fe41	0.0983374509107679	0.5775585779525152	0.1995143782094899
Fe	Fe42	0.5996317340514762	0.5769279826415843	0.1997353457589636
Fe	Fe43	0.5989445950011224	0.0787052263763172	0.2004281548924405
Fe	Fe44	0.0989769750096000	0.0783772188321262	0.1994000937409950
Fe	Fe45	0.2766172246623422	0.6679799273890576	0.2243241824059483
Fe	Fe46	0.7793248560208527	0.1684121732859059	0.2229430893905054
Fe	Fe47	0.7787513072945301	0.6674070250883337	0.2233229729325179
Fe	Fe48	0.2793276267906289	0.1705870931221427	0.2232696453549504
Fe	Fe49	0.4641017219149219	0.2606036412220510	0.2434858164380253
Fe	Fe50	0.9623414997110090	0.7596012191351448	0.2429570404519939
Fe	Fe51	0.9626887385471178	0.2602086696859363	0.2429853441909308
Fe	Fe52	0.4579709502095815	0.7583441589745064	0.2396542715620189
Fe	Fe53	0.1474522432036403	0.8536936592297556	0.2607812897670186
Fe	Fe54	0.1487533515148143	0.3513898012851572	0.2613655414110915
Fe	Fe55	0.6513699191947401	0.8547301414739841	0.2606967438035127
Fe	Fe56	0.6469150589299382	0.3499131629983165	0.2616384944522304
Fe	Fe57	0.8374197161725401	0.4467756614022442	0.2794897591574179
Fe	Fe58	0.3397057730410887	0.4461485022923692	0.2806236526744613
Fe	Fe59	0.8366401657228117	0.9472520331979428	0.2796240459639214
Fe	Fe60	0.3365960644135067	0.9555949943866333	0.2798103747073685
Fe	Fe61	0.5218334293316143	0.0263277451065020	0.2993210121831182
Fe	Fe62	0.0279072691056685	0.0432722888840304	0.2974400799798015
Fe	Fe63	0.0288519126904554	0.5428771901566867	0.2976947717301258
Fe	Fe64	0.5258605644665360	0.5518600340900623	0.2979879644983521

N N65 0.5414298865761089 0.8010094598885530 0.3172084264905387

H H66 0.4497752532069307 0.6772327837020549 0.3235758228982734

8.9 HN+H hydrogenation.cif

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Fe Fe3 0.2800 0.6687 0.0000

Fe Fe4 0.7800 0.1687 0.0000

Fe Fe5 0.4618 0.7596 0.0200

Fe Fe6 0.9618 0.2596 0.0200

Fe Fe7 0.9618 0.7596 0.0200

Fe Fe8 0.4618 0.2596 0.0200

Fe Fe9 0.6436 0.3505 0.0399

Fe Fe10 0.1436 0.8505 0.0399

Fe	Fe11	0.6436	0.8505	0.0399
Fe	Fe12	0.1436	0.3505	0.0399
Fe	Fe13	0.3255	0.4414	0.0598
Fe	Fe14	0.8255	0.9414	0.0598
Fe	Fe15	0.8255	0.4414	0.0598
Fe	Fe16	0.3255	0.9414	0.0598
Fe	Fe17	0.0073	0.0323	0.0798
Fe	Fe18	0.5073	0.0323	0.0798
Fe	Fe19	0.0073	0.5323	0.0798
Fe	Fe20	0.5073	0.5323	0.0798
Fe	Fe21	0.6891	0.1232	0.0997
Fe	Fe22	0.1891	0.6232	0.0997
Fe	Fe23	0.1891	0.1232	0.0997
Fe	Fe24	0.6891	0.6232	0.0997
Fe	Fe25	0.3709	0.2141	0.1197
Fe	Fe26	0.8709	0.2141	0.1197
Fe	Fe27	0.8709	0.7141	0.1197
Fe	Fe28	0.3709	0.7141	0.1197
Fe	Fe29	0.0527	0.8050	0.1396
Fe	Fe30	0.5527	0.8050	0.1396
Fe	Fe31	0.5527	0.3050	0.1396
Fe	Fe32	0.0527	0.3050	0.1396
Fe	Fe33	0.2345	0.8959	0.1596
Fe	Fe34	0.2345	0.3959	0.1596
Fe	Fe35	0.7345	0.8959	0.1596
Fe	Fe36	0.7345	0.3959	0.1596
Fe	Fe37	0.9164	0.4868	0.1795
Fe	Fe38	0.4164	0.4868	0.1795
Fe	Fe39	0.4164	0.9868	0.1795
Fe	Fe40	0.9164	0.9868	0.1795
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Fe	Fe43	0.5989371013610572	0.0781427473253246	0.1995431248303041

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Fe	Fe45	0.2785871099332661	0.6666456425369787	0.2236113079202766
Fe	Fe46	0.7792109674320054	0.1685090032416378	0.2234612187644589
Fe	Fe47	0.7779265373359842	0.6685853241808908	0.2242644167905005
Fe	Fe48	0.2771231140795341	0.1669456620780297	0.2228750120973462
Fe	Fe49	0.4637204691722240	0.2592934859937707	0.2457953500668391
Fe	Fe50	0.9620184361775742	0.7597715393827547	0.2426800011939110
Fe	Fe51	0.9623280967373632	0.2596458016564108	0.2427634988201790
Fe	Fe52	0.4636975510548007	0.7590510171386350	0.2426963496206025
Fe	Fe53	0.1481062652392320	0.8518034166298246	0.2604904264855499
Fe	Fe54	0.1490829268496420	0.3546379866670394	0.2615499979239011
Fe	Fe55	0.6509280364243377	0.8547056702235669	0.2607018640583759
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Fe	Fe57	0.8381521799248354	0.4474080333426450	0.2800986246796706
Fe	Fe58	0.3360666624974269	0.4466074919686842	0.2789909360003350
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Fe	Fe60	0.3365005668821093	0.9427084318976025	0.2793006946406762
Fe	Fe61	0.5243694096647268	0.0385979547165648	0.2966064220546510
Fe	Fe62	0.0273599761879178	0.0423662630314183	0.2974306967950051
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Fe	Fe64	0.5359011268911218	0.5515842227794783	0.2993857368960122
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H	H66	0.4269865414534086	0.1936950077993883	0.3198129041972904
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8.10 H_2N+H hydrogenation.cif

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Fe	Fe4	0.7800	0.1687	0.0000
Fe	Fe5	0.4618	0.7596	0.0200
Fe	Fe6	0.9618	0.2596	0.0200
Fe	Fe7	0.9618	0.7596	0.0200
Fe	Fe8	0.4618	0.2596	0.0200
Fe	Fe9	0.6436	0.3505	0.0399
Fe	Fe10	0.1436	0.8505	0.0399
Fe	Fe11	0.6436	0.8505	0.0399
Fe	Fe12	0.1436	0.3505	0.0399
Fe	Fe13	0.3255	0.4414	0.0598
Fe	Fe14	0.8255	0.9414	0.0598
Fe	Fe15	0.8255	0.4414	0.0598
Fe	Fe16	0.3255	0.9414	0.0598
Fe	Fe17	0.0073	0.0323	0.0798
Fe	Fe18	0.5073	0.0323	0.0798
Fe	Fe19	0.0073	0.5323	0.0798
Fe	Fe20	0.5073	0.5323	0.0798
Fe	Fe21	0.6891	0.1232	0.0997

Fe	Fe22	0.1891	0.6232	0.0997
Fe	Fe23	0.1891	0.1232	0.0997
Fe	Fe24	0.6891	0.6232	0.0997
Fe	Fe25	0.3709	0.2141	0.1197
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Fe	Fe28	0.3709	0.7141	0.1197
Fe	Fe29	0.0527	0.8050	0.1396
Fe	Fe30	0.5527	0.8050	0.1396
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Fe	Fe33	0.2345	0.8959	0.1596
Fe	Fe34	0.2345	0.3959	0.1596
Fe	Fe35	0.7345	0.8959	0.1596
Fe	Fe36	0.7345	0.3959	0.1596
Fe	Fe37	0.9164	0.4868	0.1795
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Fe	Fe40	0.9164	0.9868	0.1795
Fe	Fe41	0.0989738636004871	0.5766390283725289	0.1998830590800789
Fe	Fe42	0.5981767978430425	0.5777570651353620	0.2010895116236656
Fe	Fe43	0.5995076560805553	0.0783949633772116	0.1995169706783459
Fe	Fe44	0.0989846197854156	0.0796869627392581	0.1998897935175144
Fe	Fe45	0.2786097408016016	0.6671564171844687	0.2234351034551801
Fe	Fe46	0.7790110236035198	0.1682395056974535	0.2236916262738688
Fe	Fe47	0.7781336609359163	0.6678224347037881	0.2232176598936699
Fe	Fe48	0.2786081038869390	0.1688791876291373	0.2234260111738172
Fe	Fe49	0.4627611442152464	0.2591563361276583	0.2416873147174402
Fe	Fe50	0.9623060544624281	0.7598446011685376	0.2424344434586730
Fe	Fe51	0.9627848424009459	0.2600983103937223	0.2428304660930257
Fe	Fe52	0.4627738945358608	0.7609203727760255	0.2417110362369115
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Fe	Fe55	0.6480119753648443	0.8502701274948570	0.2614372885302761
Fe	Fe56	0.6480200829023046	0.3549715476168057	0.2614251536189471
Fe	Fe57	0.8368442751691825	0.4475626644441671	0.2797524941082543
Fe	Fe58	0.3362171269213149	0.4467881001519546	0.2787069341380378
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Fe	Fe61	0.5271117371180256	0.0423156180082354	0.2966718566867932
Fe	Fe62	0.0264258593135926	0.0421542565352463	0.2971286162461345
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Fe	Fe64	0.5188668037695519	0.5380598104750380	0.3010946045447946
N	N65	0.4033414018923409	0.4803723286448893	0.3665139435545863
H	H66	0.2999633901938148	0.4286566016075152	0.3514185203701767
H	H67	0.4034418043410548	0.5847266591030362	0.3943118380357898
H	H68	0.4034138180510321	0.3761714003054812	0.3943562624194705